

Diffrazione di raggi X, diffrazione da superfici

Per approfondimenti:

1. **E. Vlieg**
X-Ray Diffraction from Surfaces and Interfaces

<https://onlinelibrary.wiley.com/doi/10.1002/9783527680535.ch10>

2. **Surface Science Reports 10 (1989) 105–188** 105
North-Holland, Amsterdam

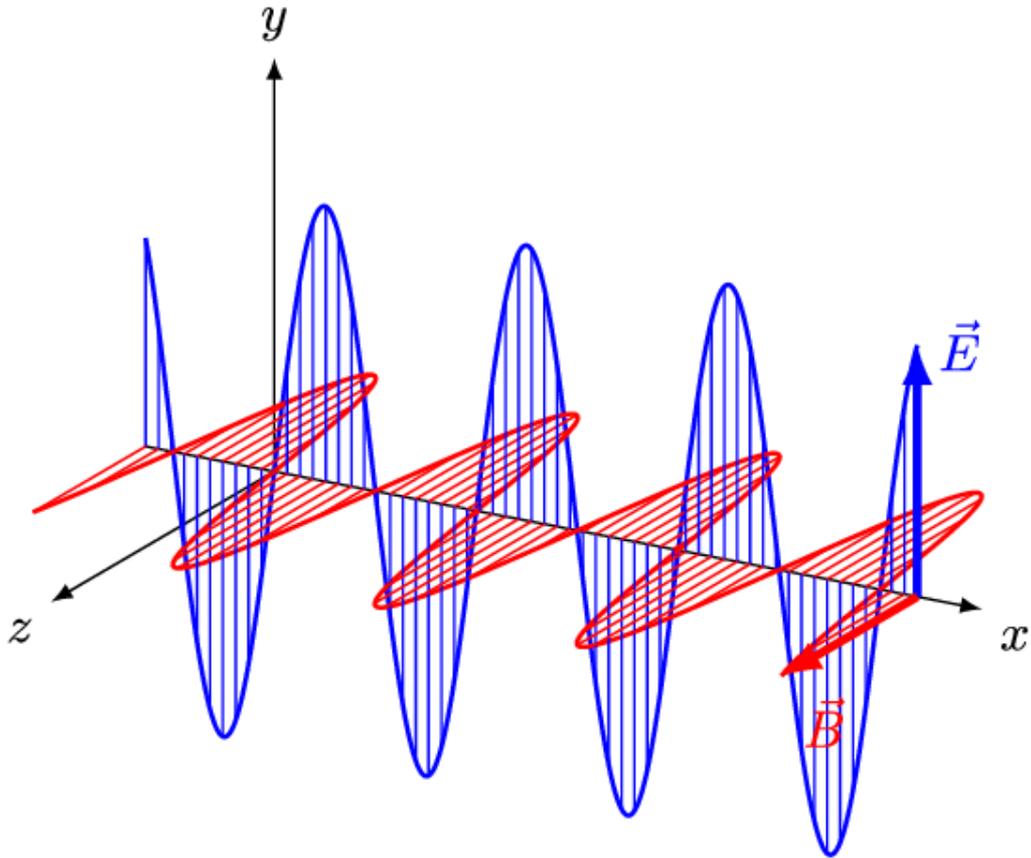
SURFACE STRUCTURE DETERMINATION BY X-RAY DIFFRACTION

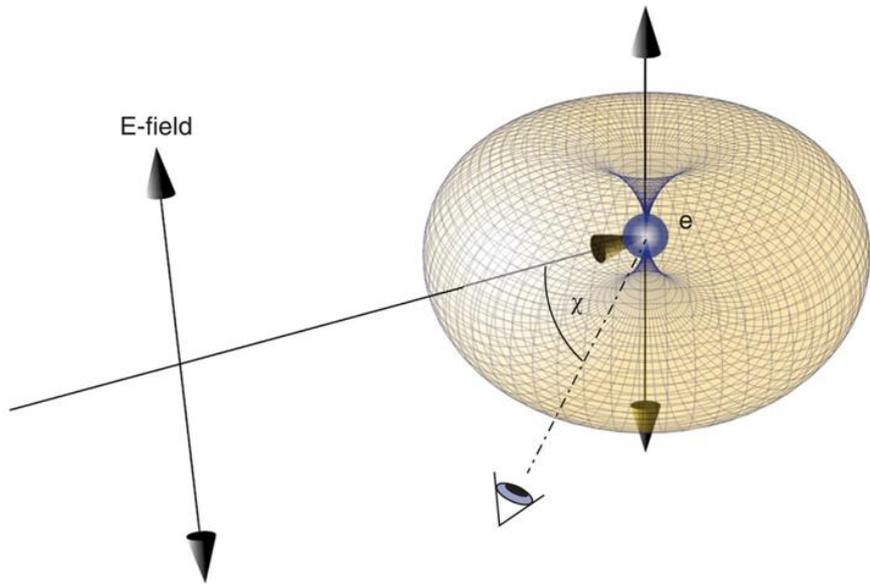
R. FEIDENHANS'L

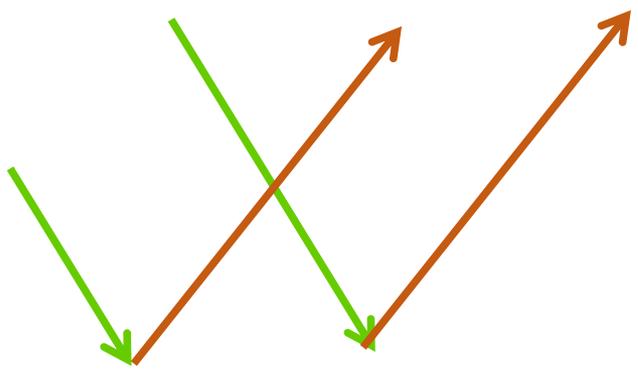
Risø National Laboratory, DK-4000, Roskilde, Denmark

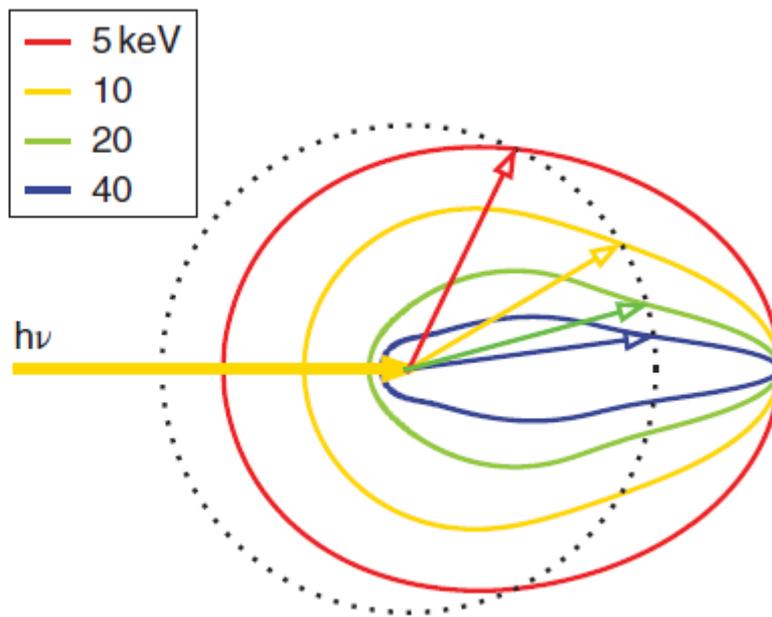
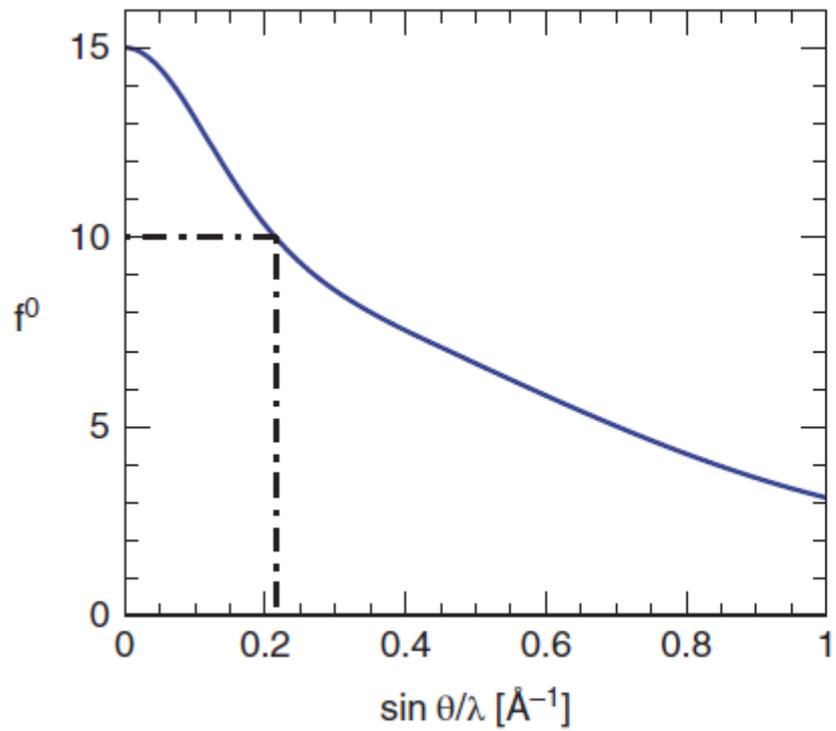
Manuscript received in final form 2 February 1989

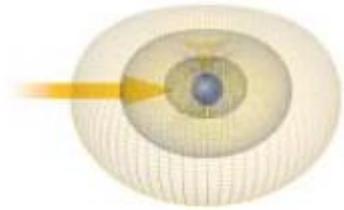
Interazione radiazione-materia



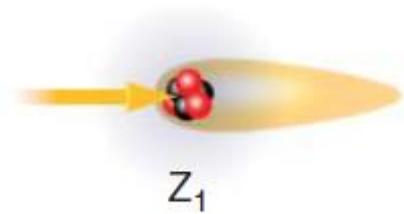




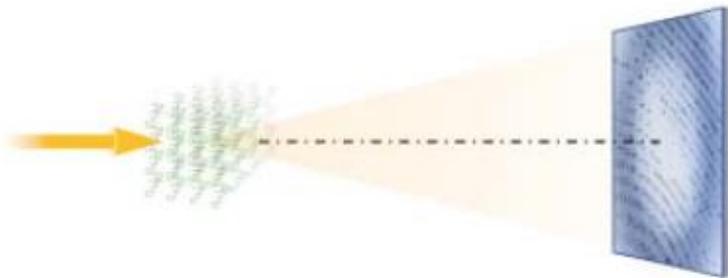




Scattering da un elettrone



Scattering da un atomo



Scattering da un cristallo

Diffrazione di raggi X

Se ho N atomi, il campo diffuso sarà la somma dei contributi di ognuno, sempre pesata per la differenza di fase:

Se gli atomi appartengono ad un reticolo cristallino, l'interferenza tra i contributi di ognuno danno origine ad un pattern di diffrazione

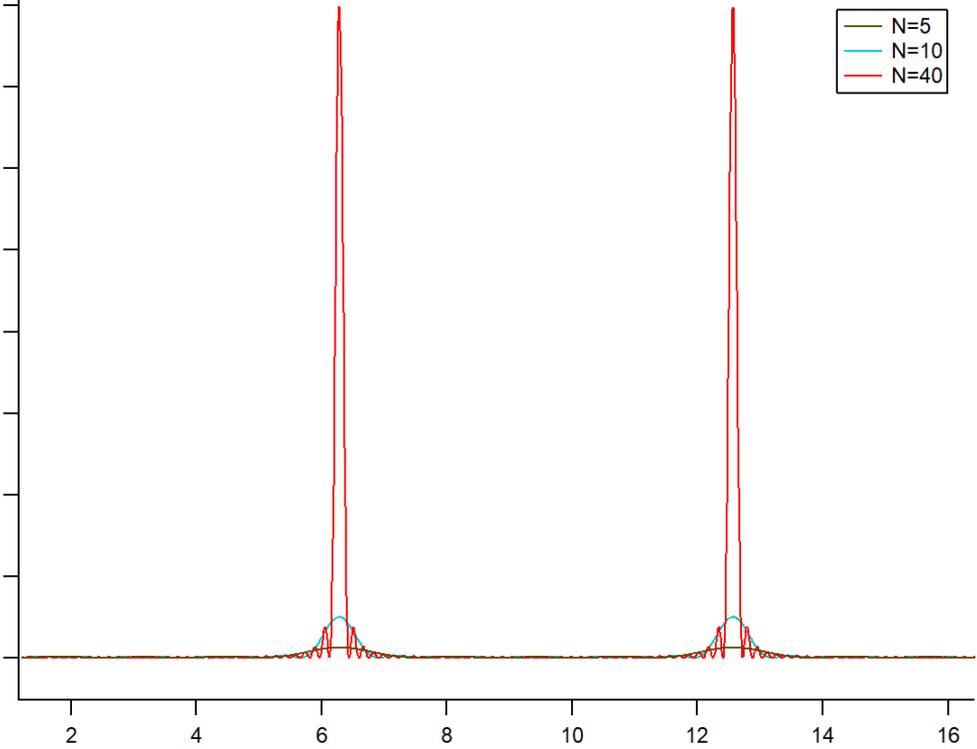
Se il cristallo è descritto da una cella primitiva con base,
scrivo prima il contributo della singola cella:



Fattore di Struttura

Se il cristallo è costituito da $N_1 \times N_2 \times N_3$ celle:

L'intensità diffratta da un cristallo sarà perciò:





L'insieme di punti \vec{q} che soddisfano le relazioni precedenti formano un reticolo, definito nello spazio \vec{k} , detto **reticolo reciproco**.

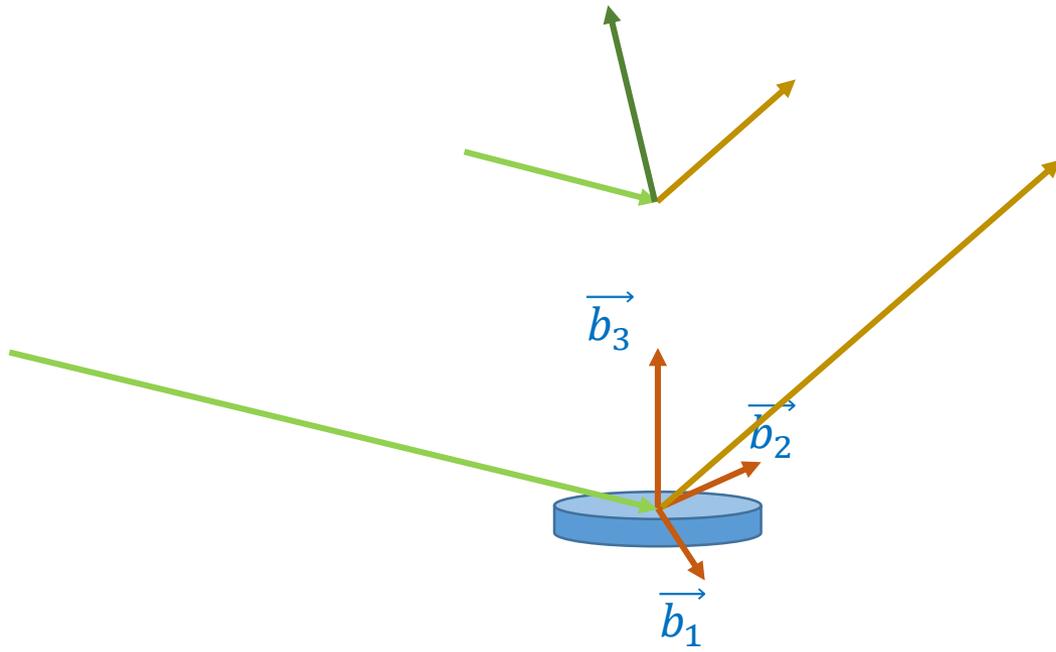
Ogni reticolo cristallino, identificato da una cella di vettori $\vec{a}_1, \vec{a}_2, \vec{a}_3$, ha associato un reticolo reciproco la cui cella è:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

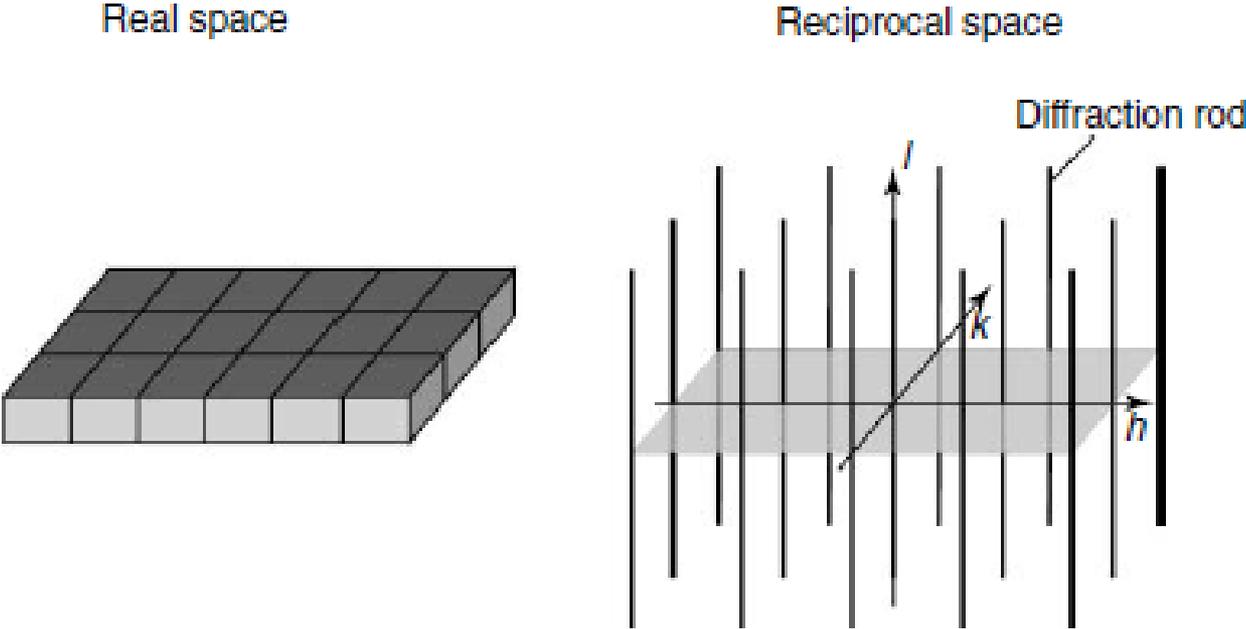
$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Nota: La cella di Wigner Seitz del reticolo reciproco è chiamata zona di Brillouin.

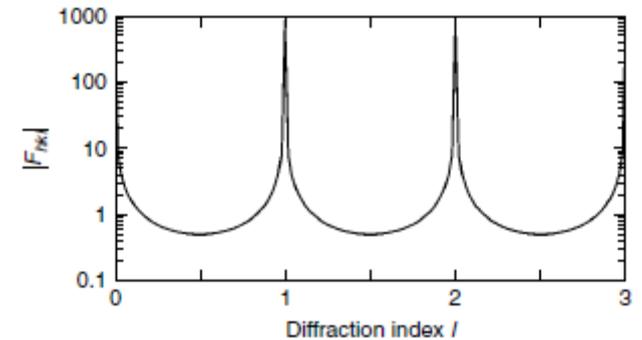
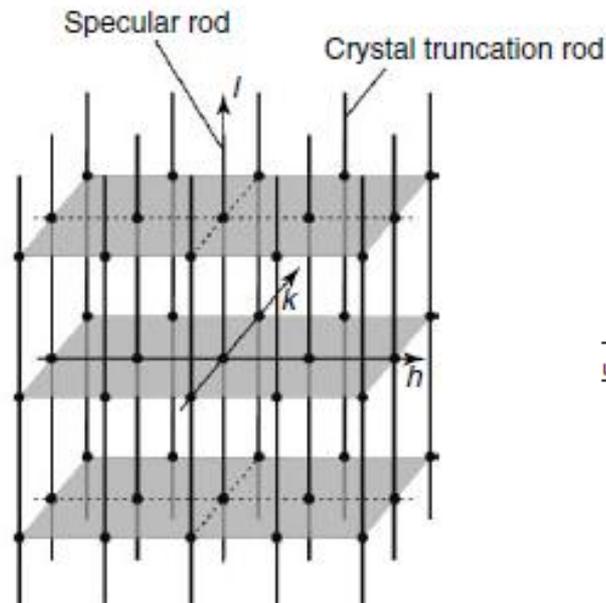
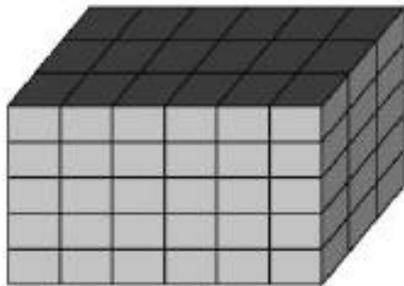


Se considero la diffrazione da un sistema 2D, le condizioni di diffrazione si applicano solo su x e y . La condizione su z scompare:

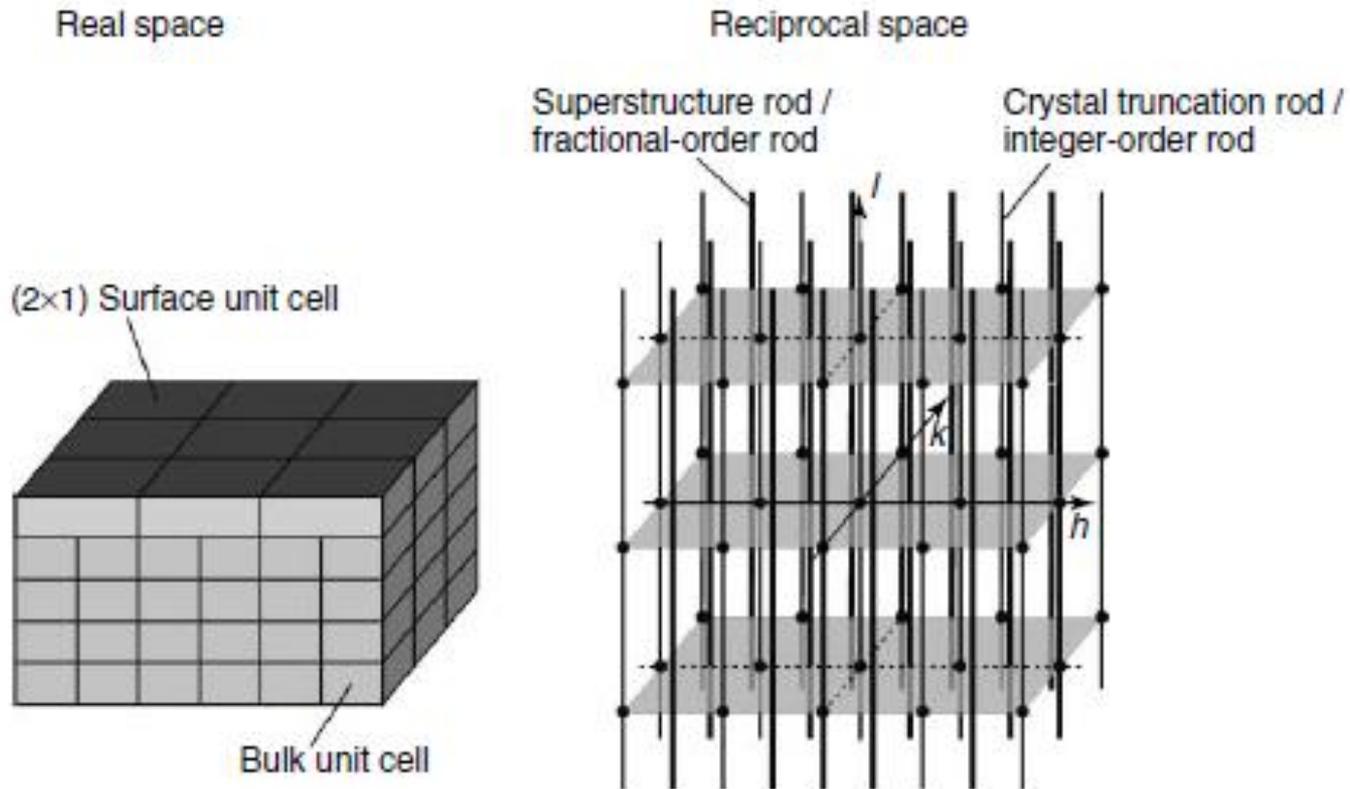
il reticolo reciproco di un sistema 2D è un insieme di rod.



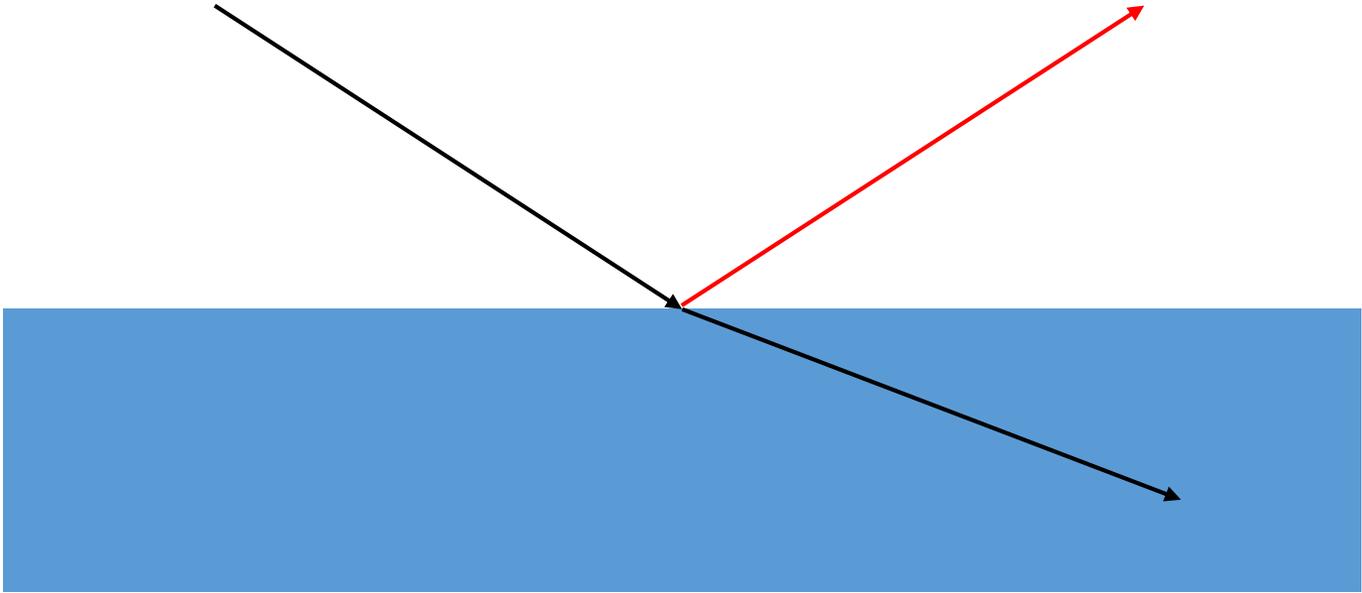
!! Un Sistema reale sarà sempre 3D. Posso vederlo come la somma di bulk + superficie.
La presenza della superficie fa sì che oltre ai picchi di diffrazione di bulk ci sia intensità diffratta anche lungo le rod.

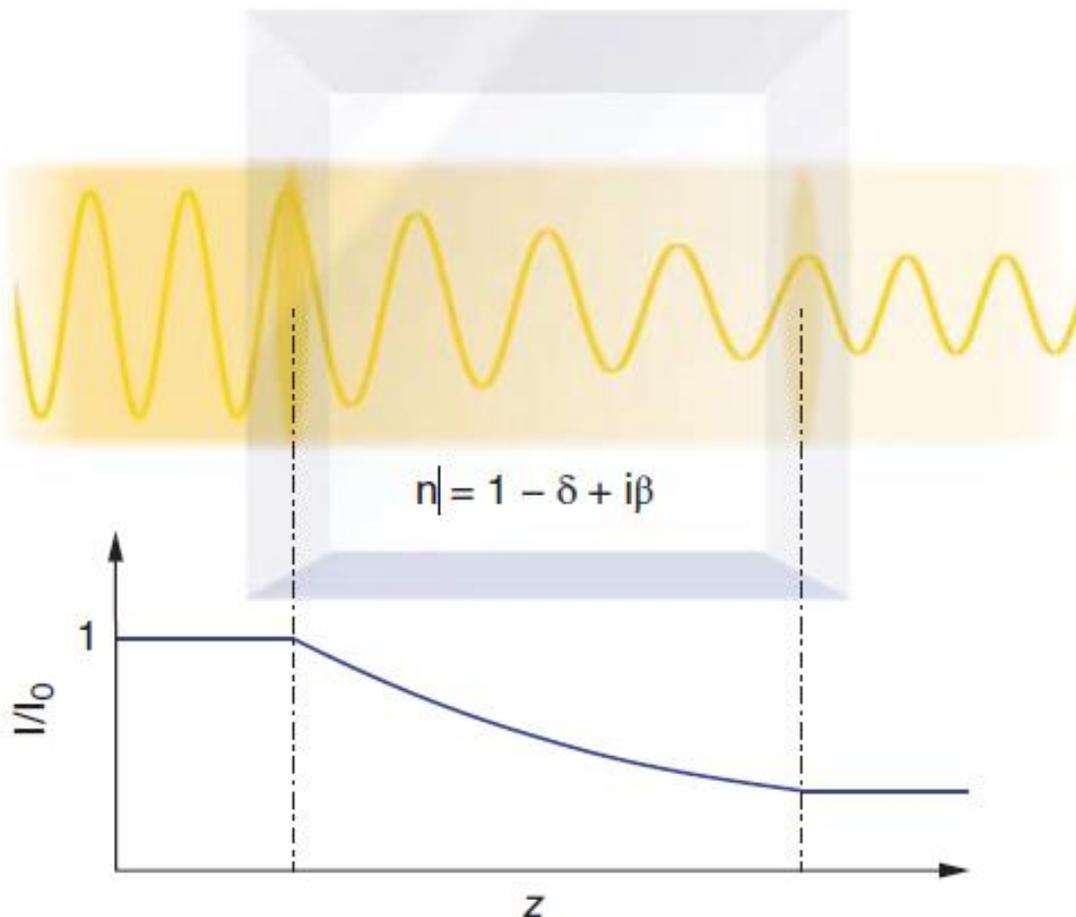


Se ho una ricostruzione della superficie, compariranno delle rod in corrispondenza di ordini frazionari.



Nella regione dei raggi X l'indice di rifrazione è:

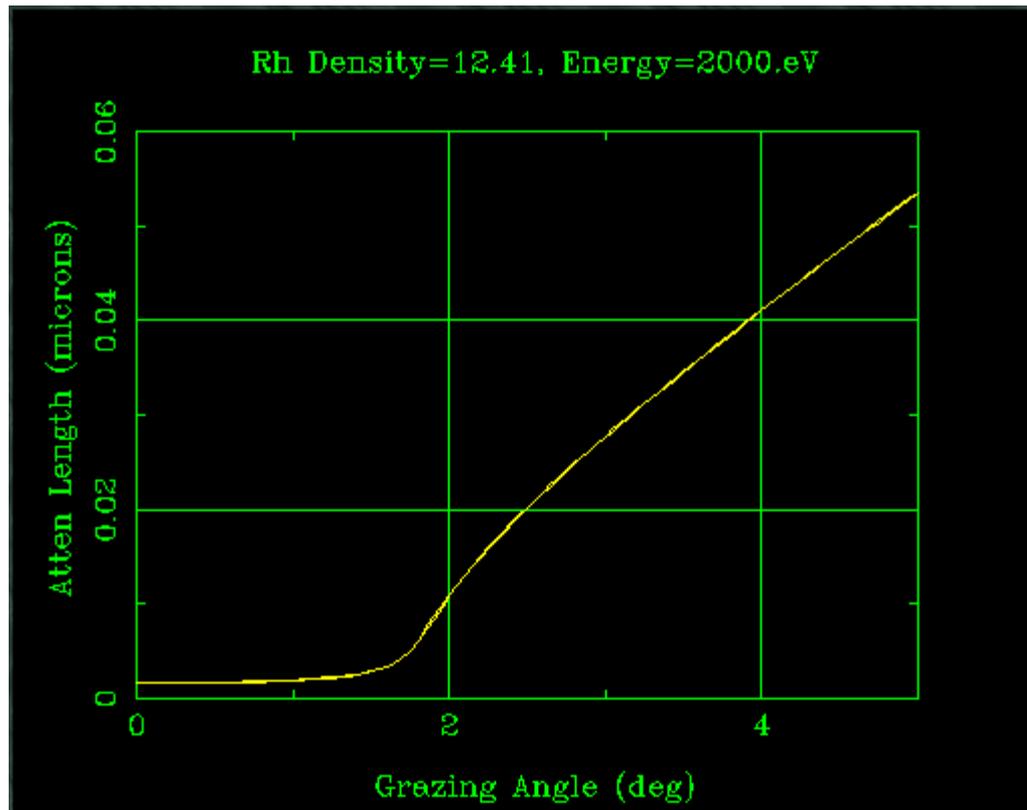




Equazione di Beer-Lambert

Si può verificare che la lunghezza di penetrazione nel mezzo è:

$$\Lambda = \frac{\lambda}{4\pi \text{Im} \sqrt{\alpha^2 - \alpha_c^2 - 2i\beta}}$$



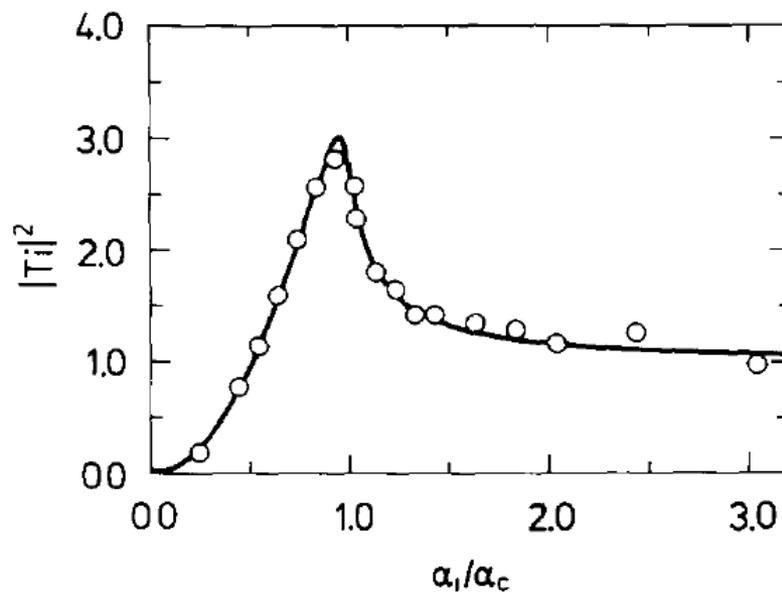
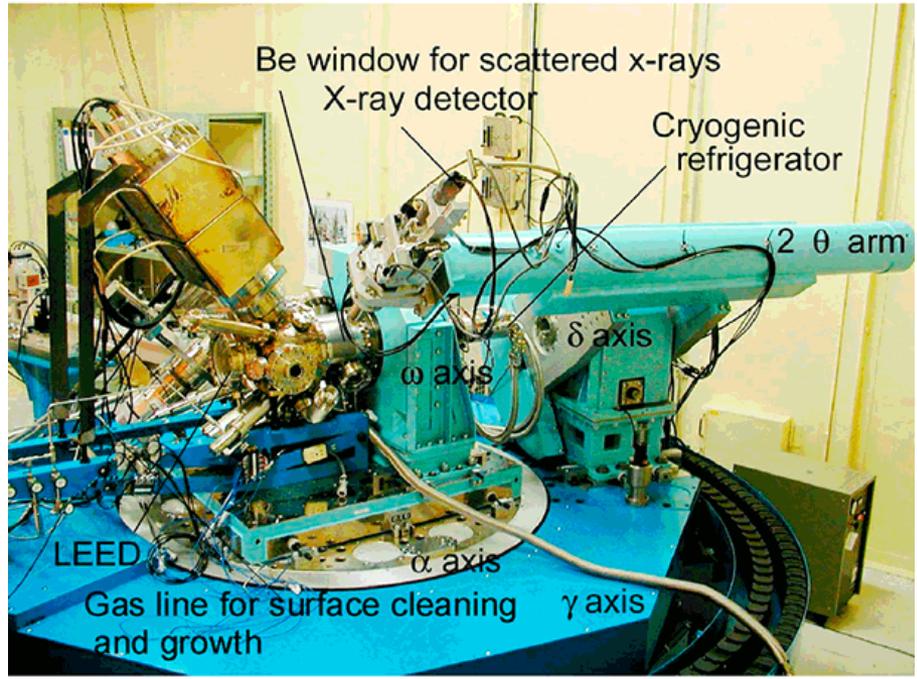
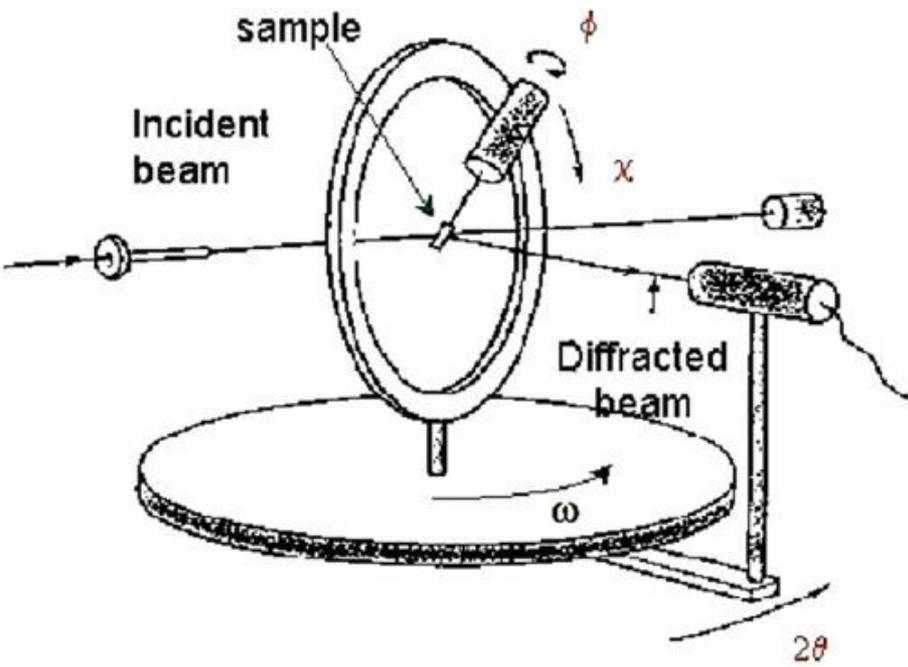
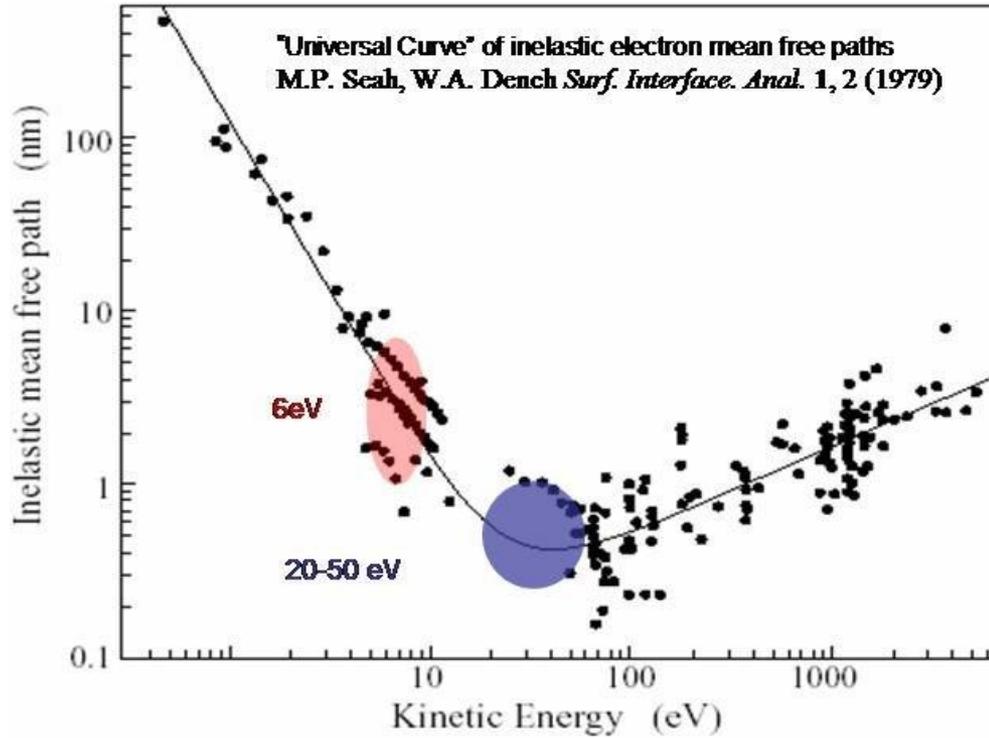


Fig. 6. Transmission coefficient $|T_i|^2$ as a function of incidence angle α_i . The curve is shown for an InSb(111) surface and a wavelength $\lambda = 1.2 \text{ \AA}$, the critical angle is $\alpha_c = 0.25^\circ$. The experimental points are from the $(4/3,0)$ reflection of the InSb($\bar{1}\bar{1}\bar{1}$) 3×3 surface normalized to the correct scale. The intensity of a superlattice reflection is a measure of the intensity of the evanescent wave and hence of the transmission coefficient. From ref. [25].



Il libero cammino medio degli **elettroni** nel mezzo è invece molto inferiore

Cammino libero medio degli elettroni nella materia



$$\lambda = \frac{143}{E^2} + 0.054 \cdot \sqrt{E}$$

LEED: Low Energy Electron Diffraction

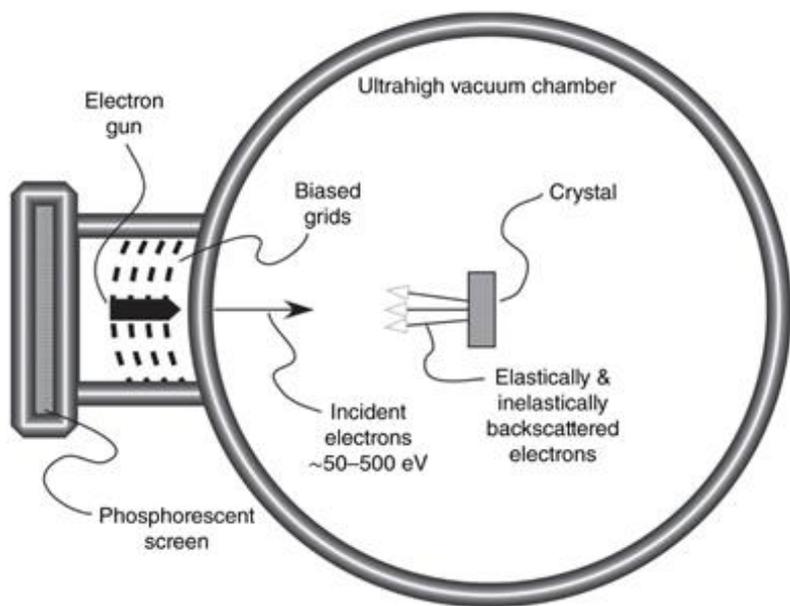
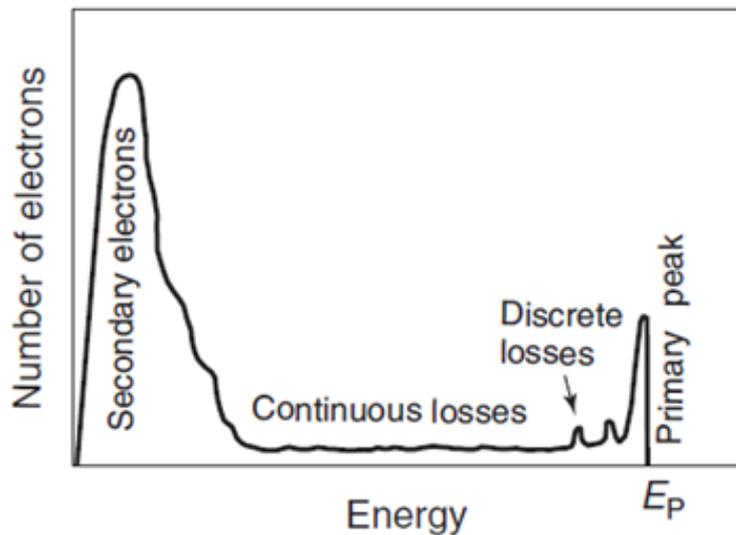
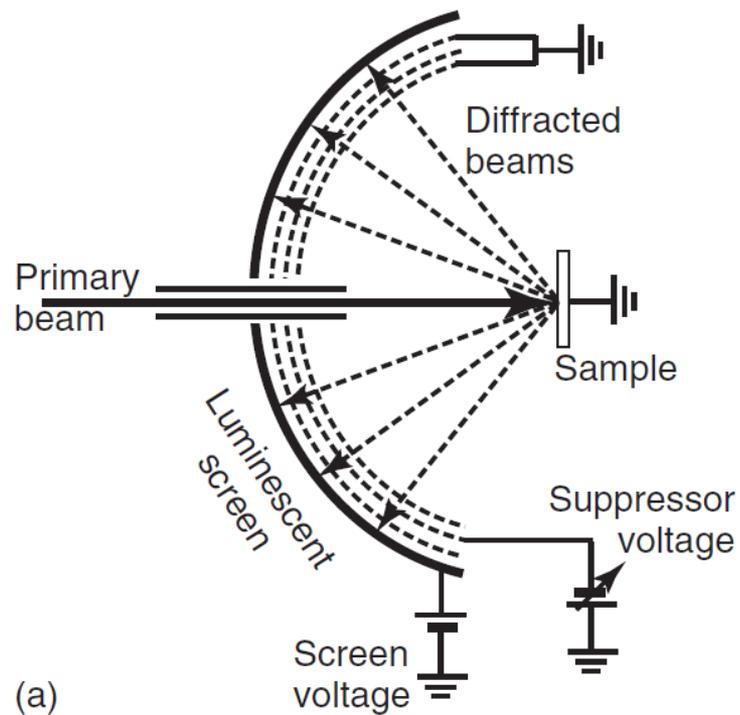


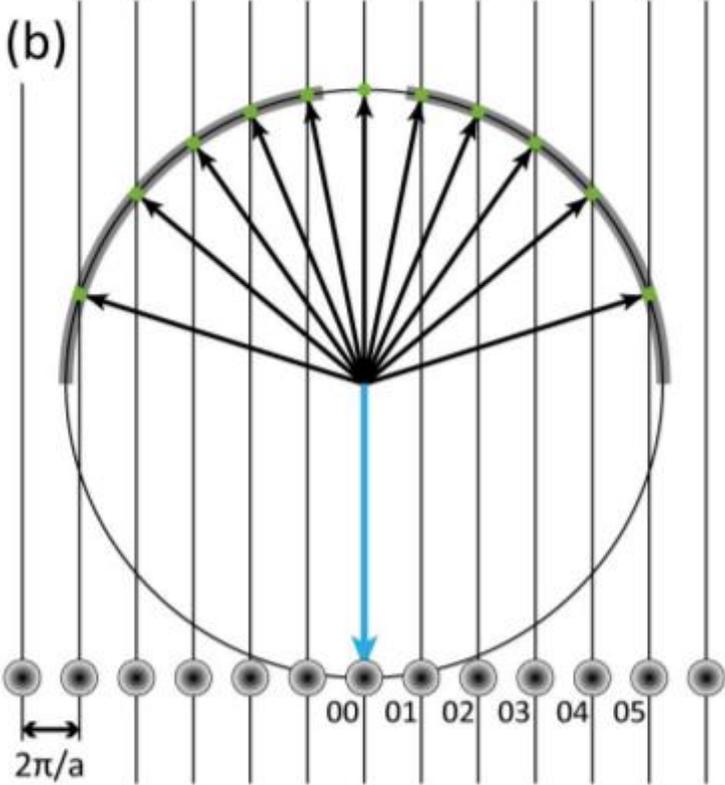
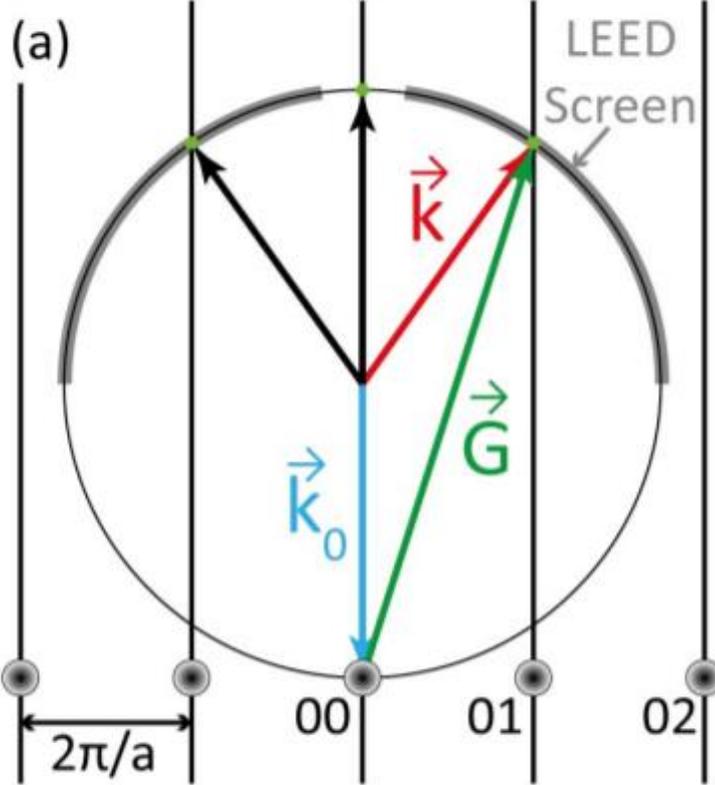
Figure 2.12 Schematic drawing of a LEED chamber.

Surface Science: Foundations of Catalysis and Nanoscience, Fourth Edition.
Kurt W. Kolasinski.
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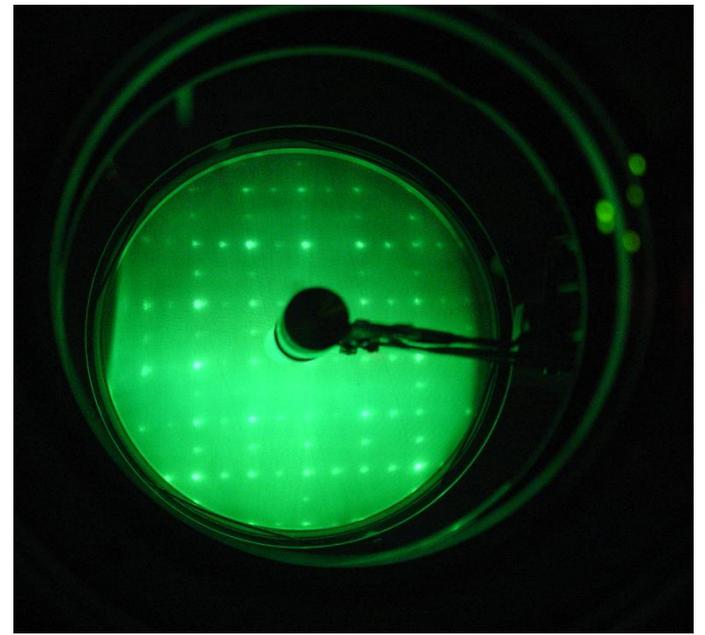
(a)

SFERA di EWALD

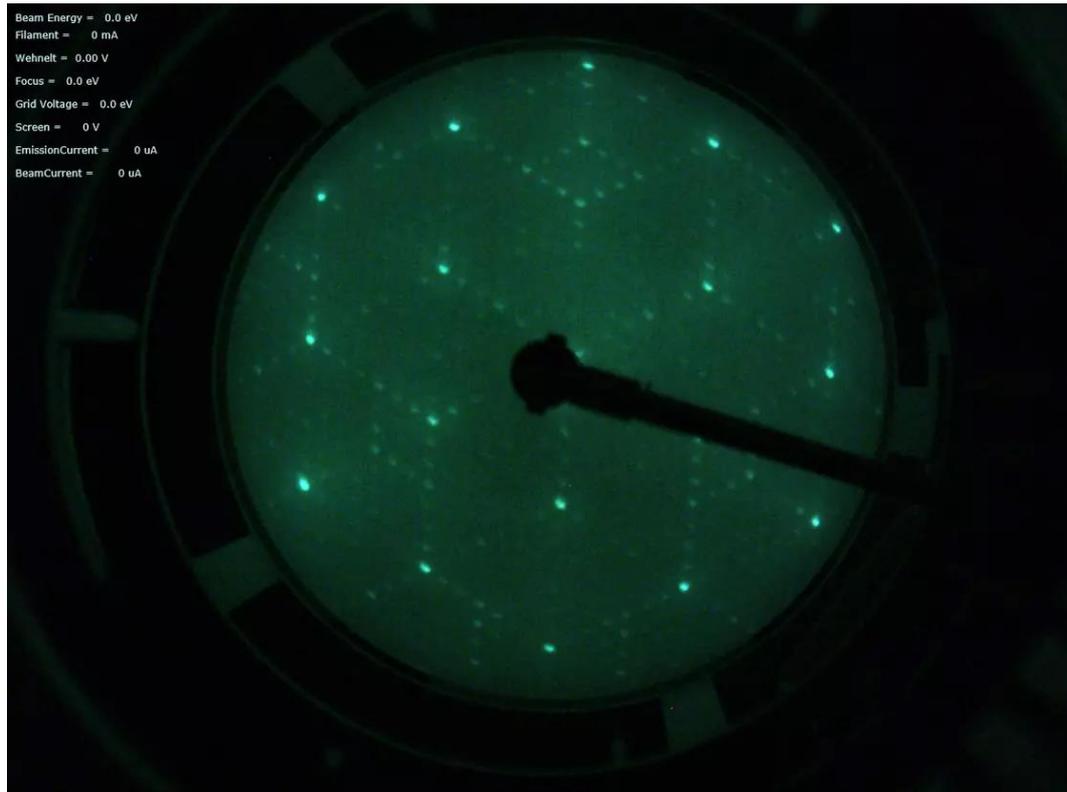




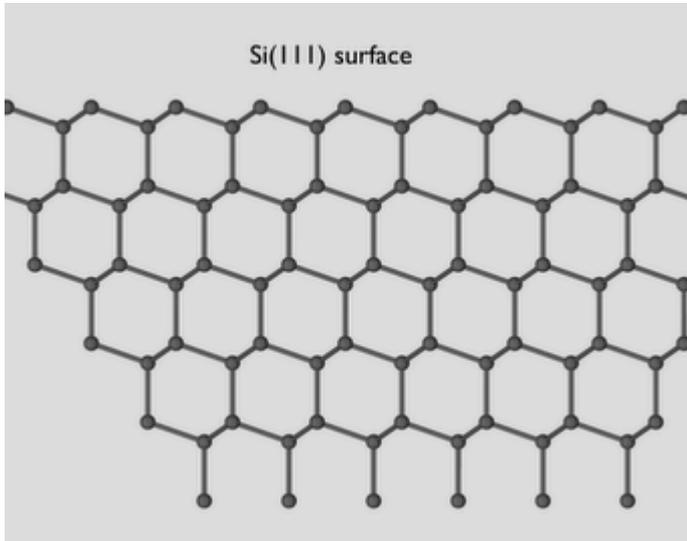
www.ocivm.com



Si (111): ricostruzione 7x7

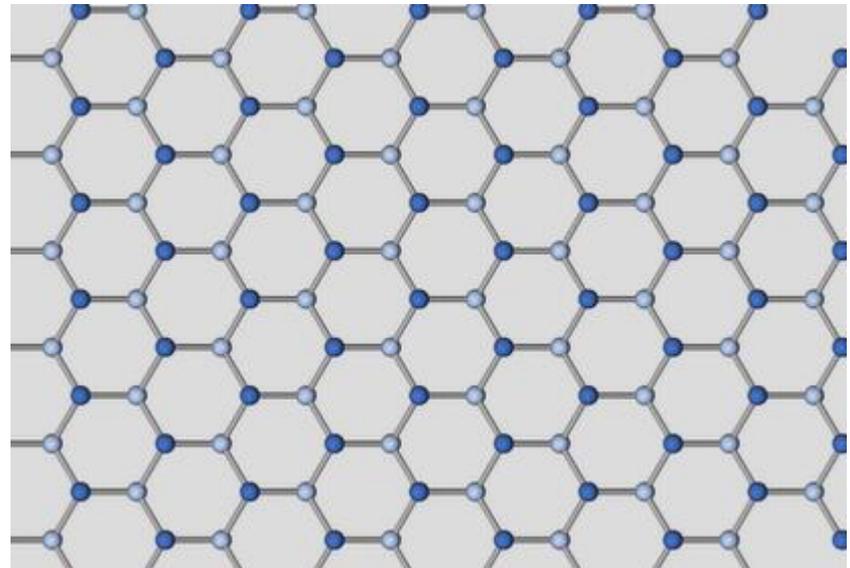
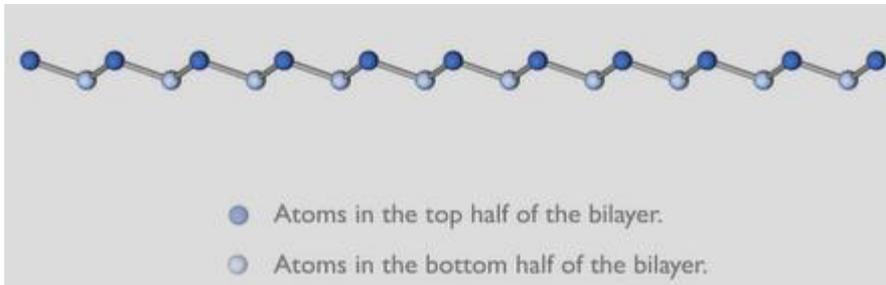


Si (111): ricostruzione 7x7

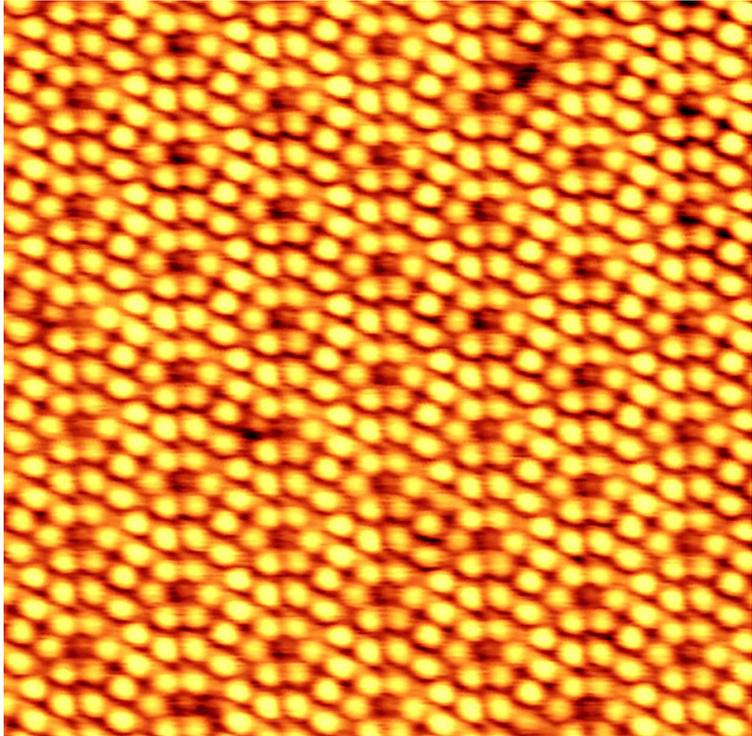
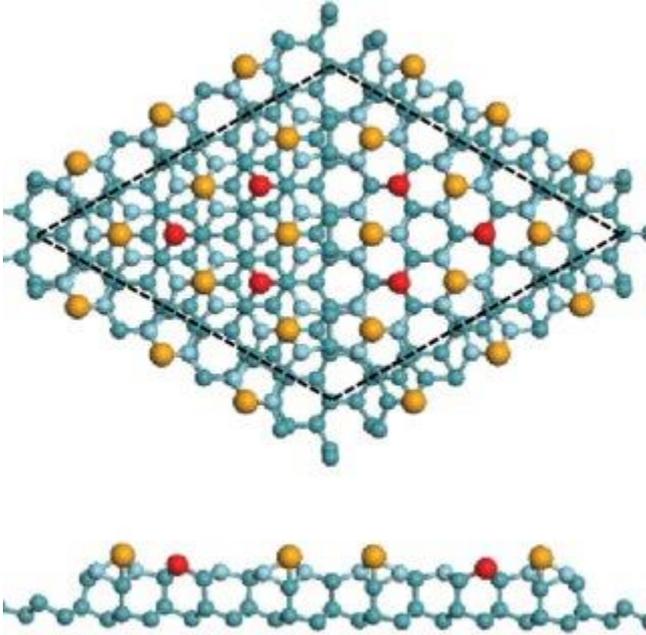


Animazione su:

<https://vimeo.com/1086112>



Si (111): ricostruzione 7x7



La superficie (110) dell'oro spontaneamente ricostruisce 1x2

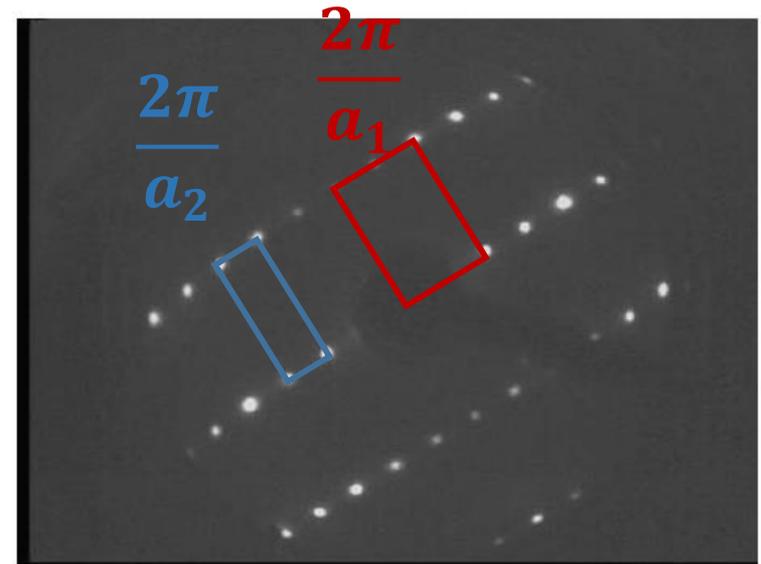
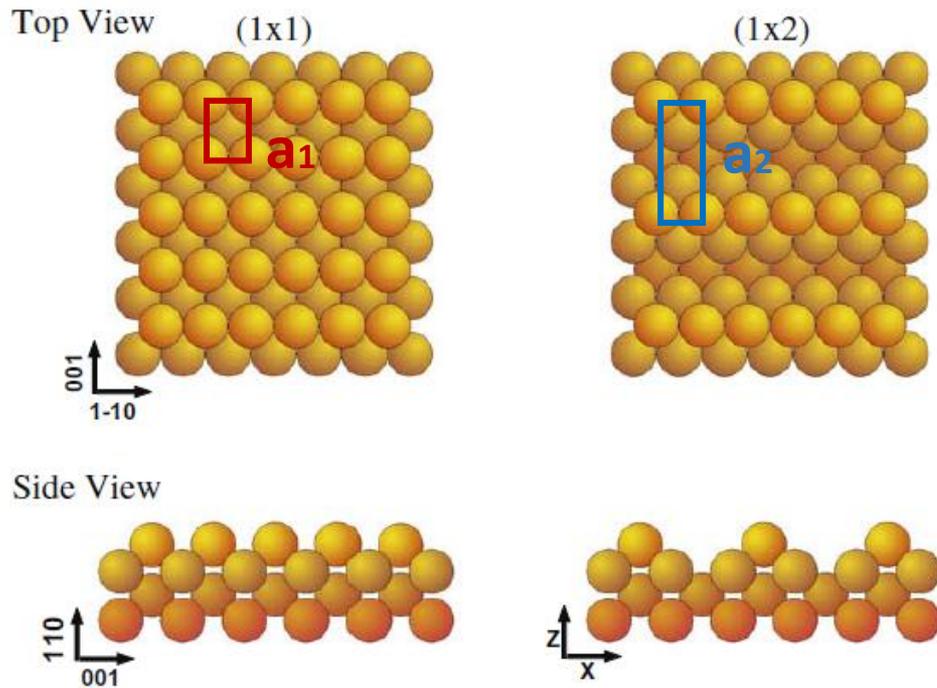
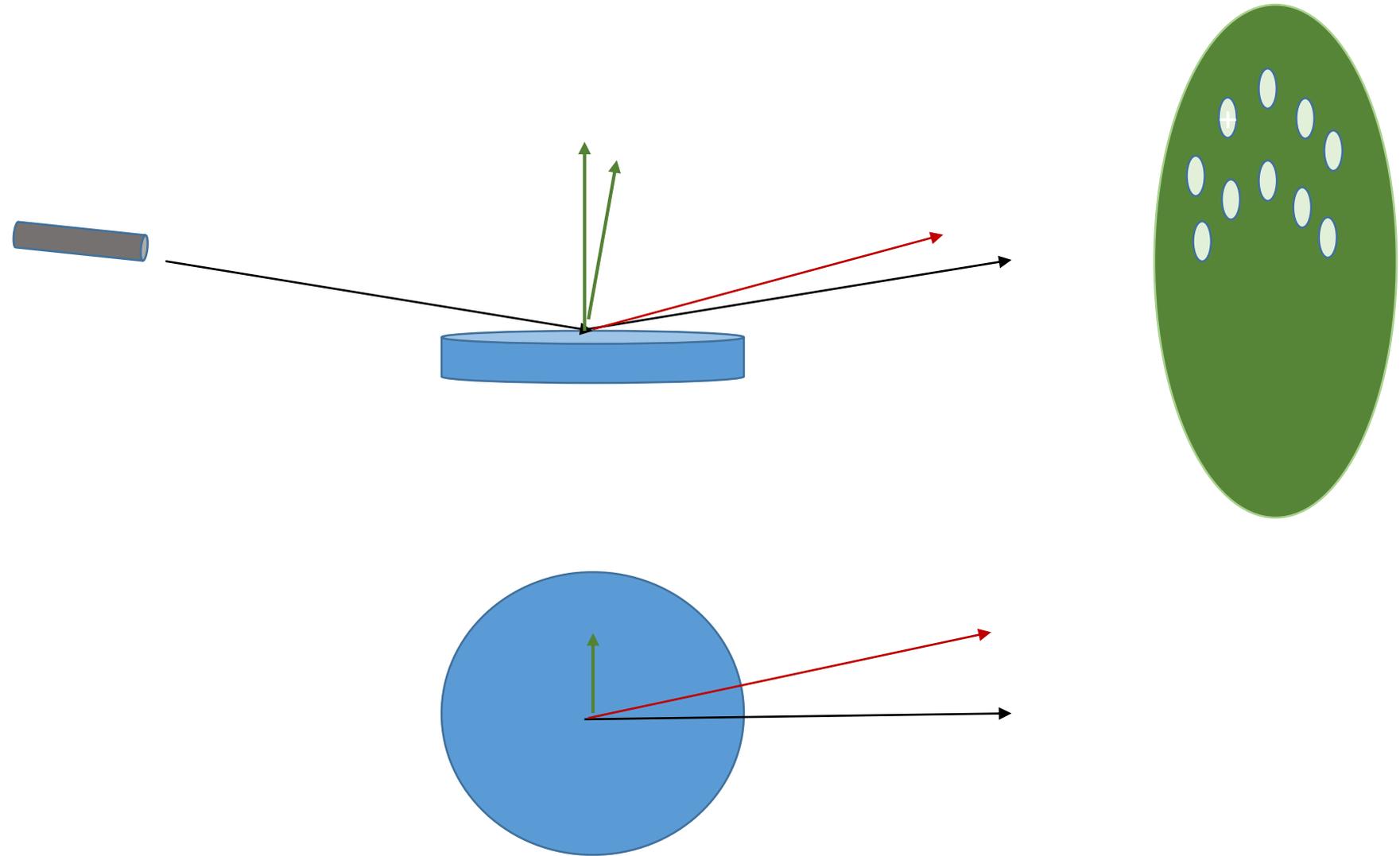


Fig. 2. LEED pattern at 130 eV

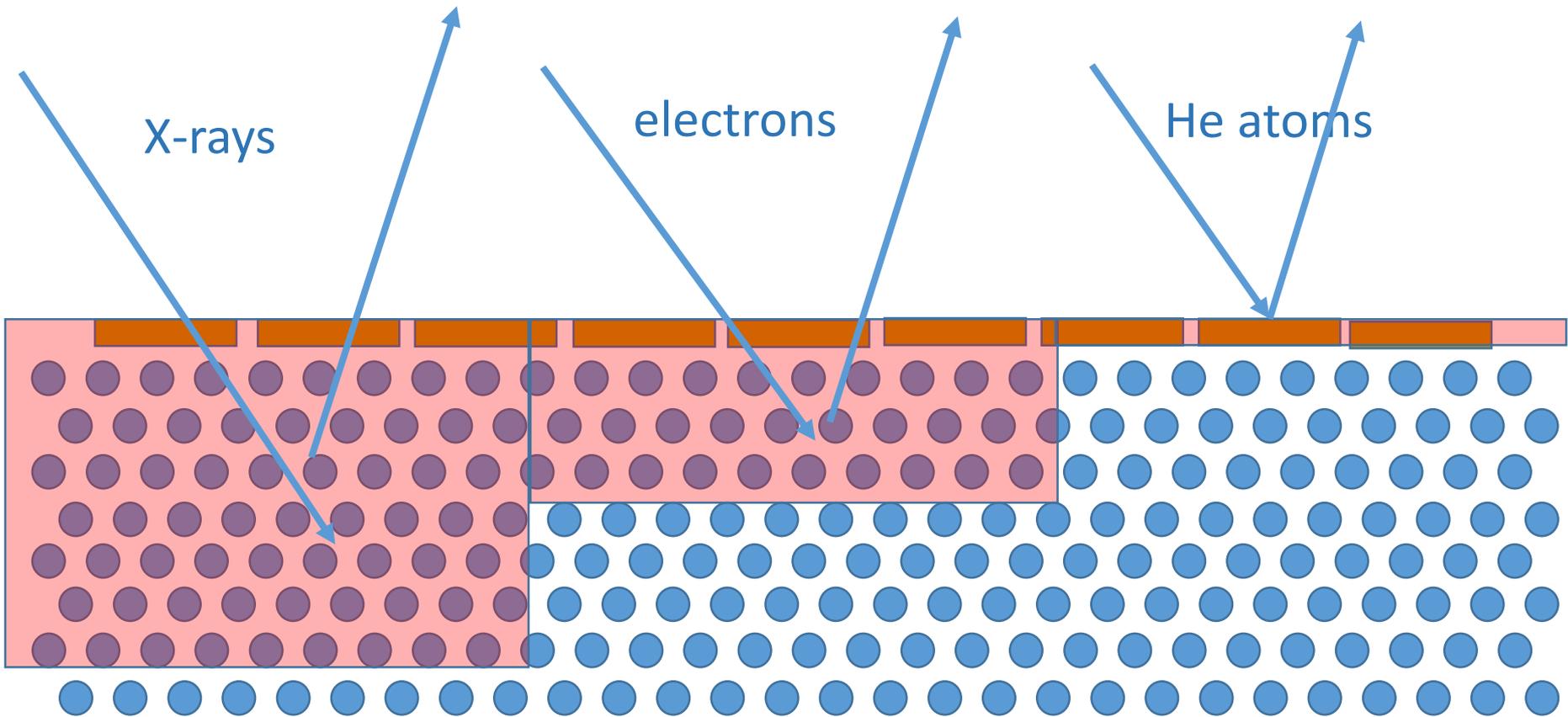
RHEED – Reflection High-Energy Electron Diffraction



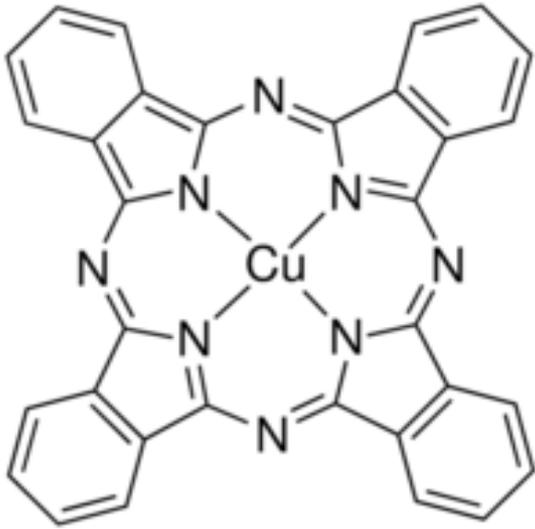
X-rays

electrons

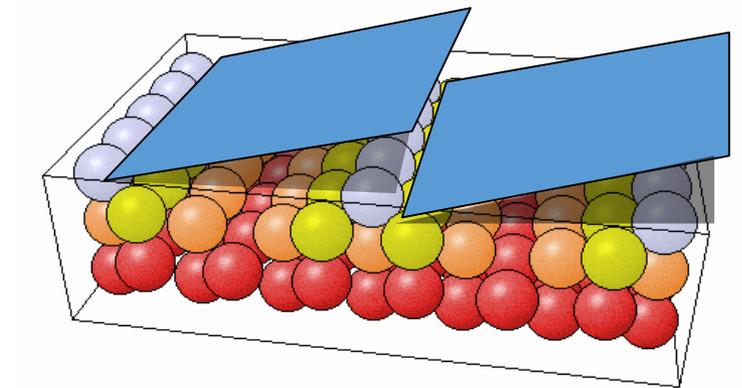
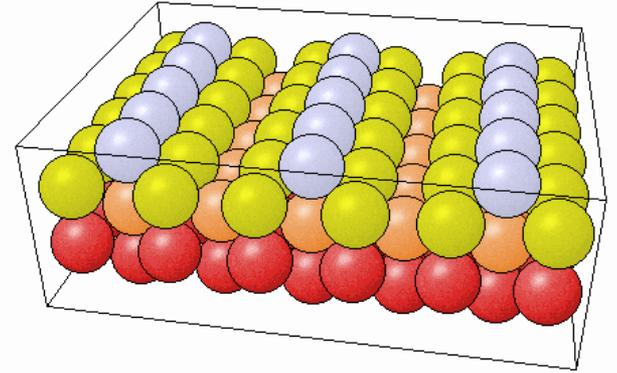
He atoms



The CuPc/Au(110) system

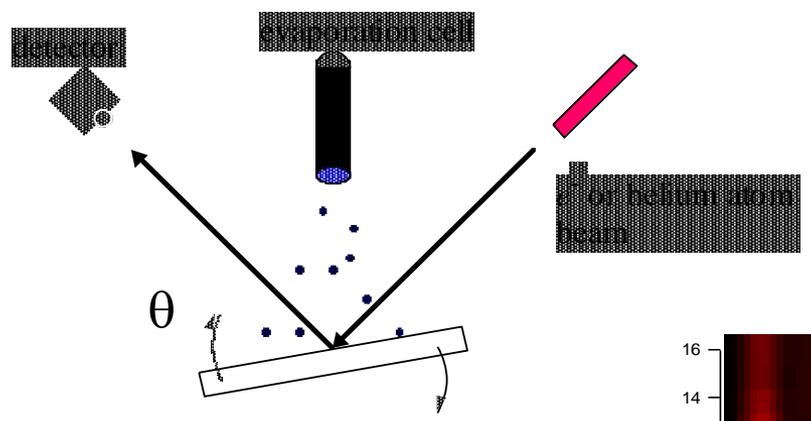


Planar shape
High thermal stability
High chemical stability

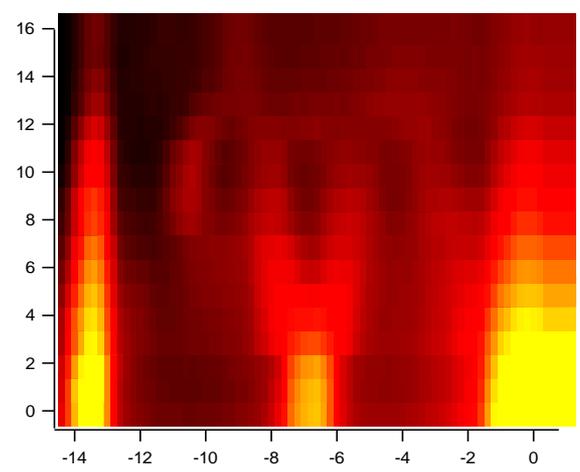


The CuPc/Au(110) system

Cu-Pc/Au(110) growth



Electron diffraction

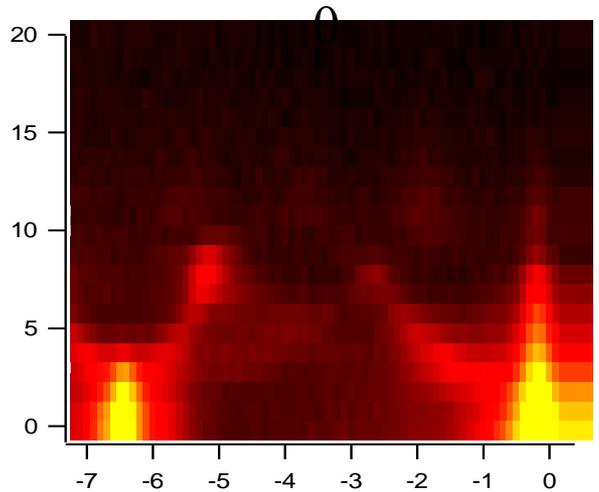


\times 3 phase

\times 5 phase

\times 2 substrate phase

He atom diffraction



\times 7 phase

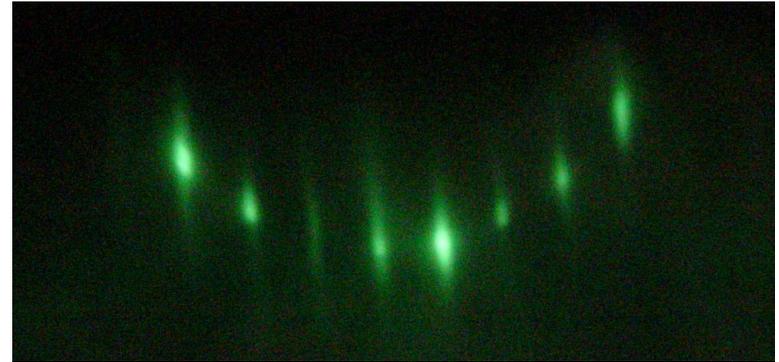
\times 5 phase

\times 2 substrate phase

The CuPc/Au(110) system

RHEED growth evolution

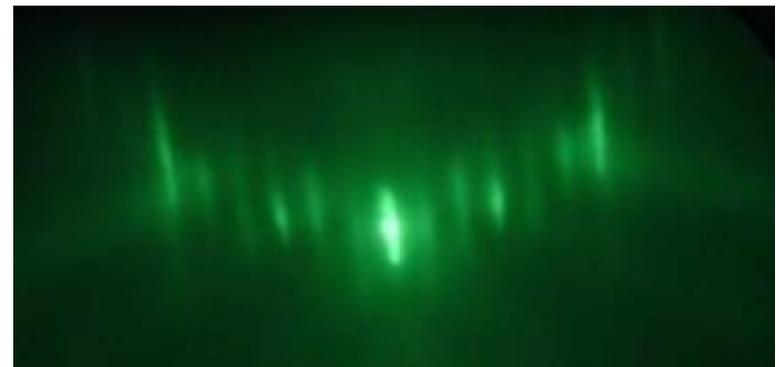
Au(110) 1x2 missing row



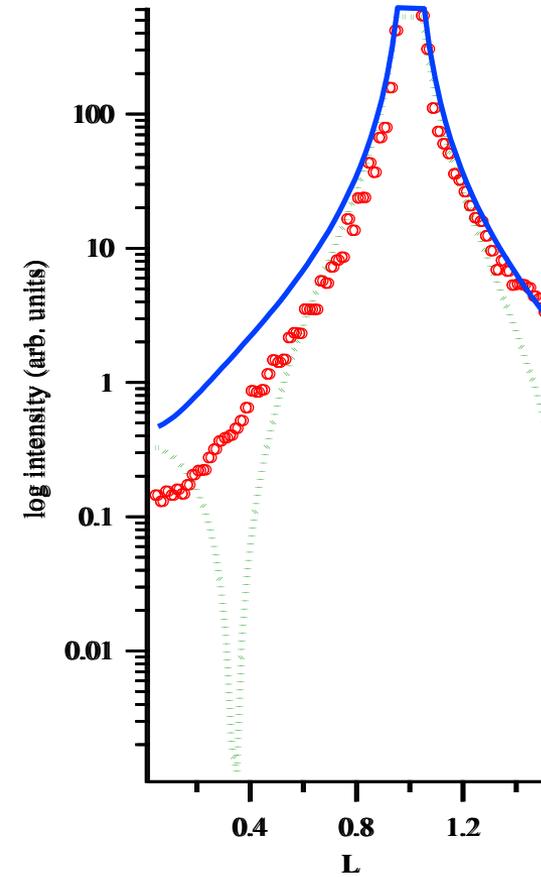
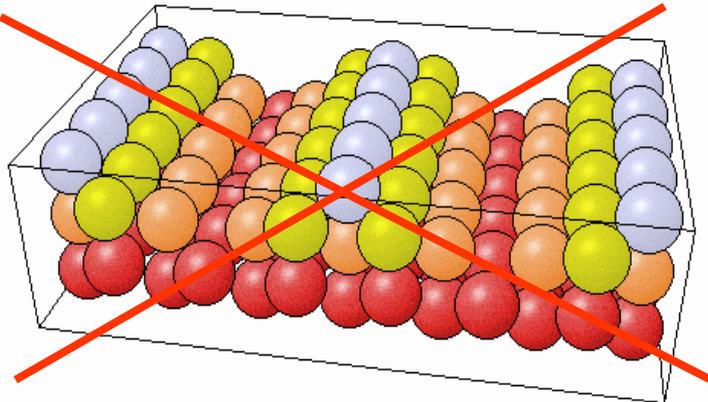
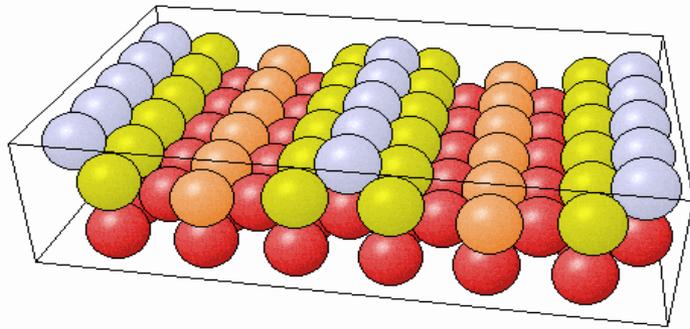
Cu-Pc / Au x5 phase

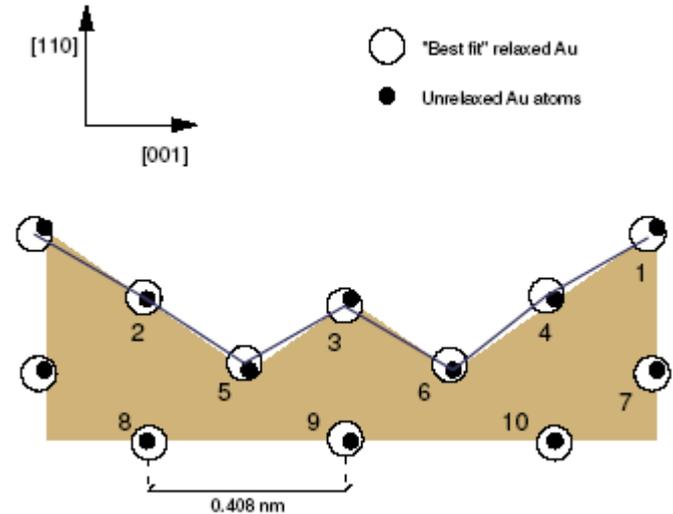
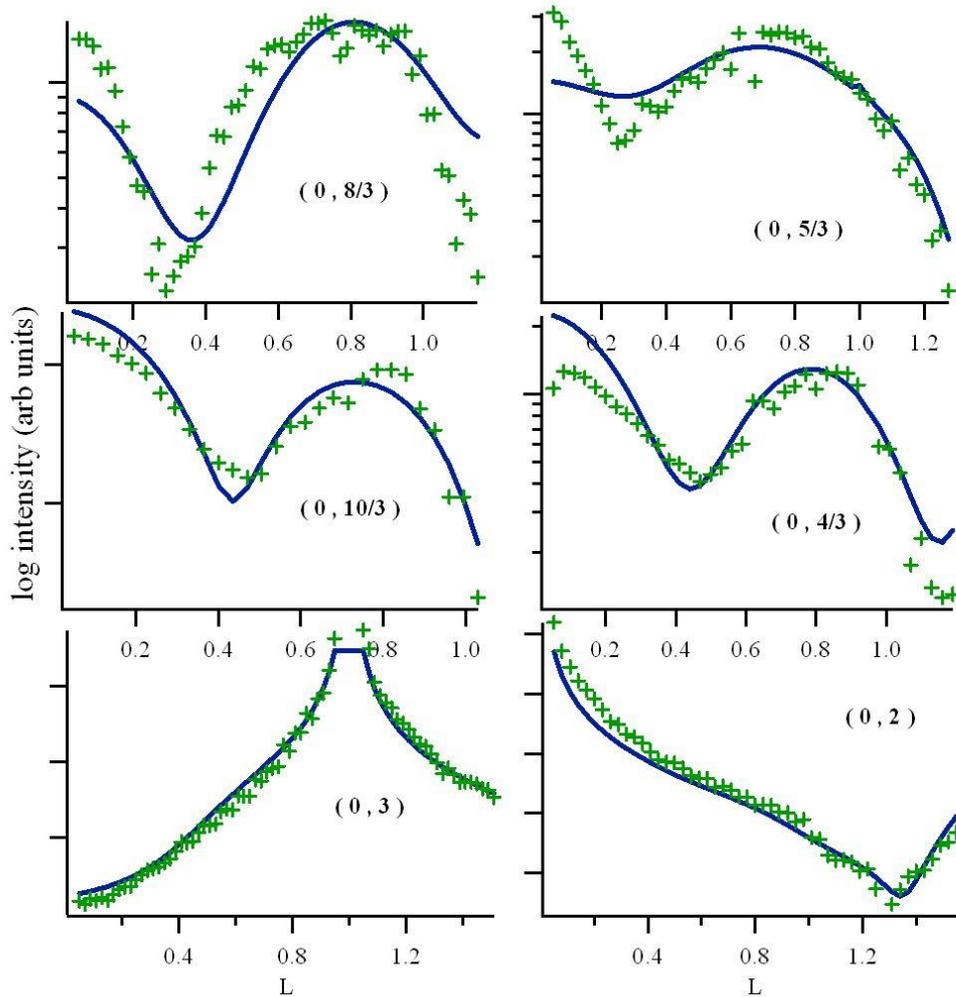


Cu-Pc / Au x3 phase



(0, 3) rods can





Shallow $\times 3$ reconstruction

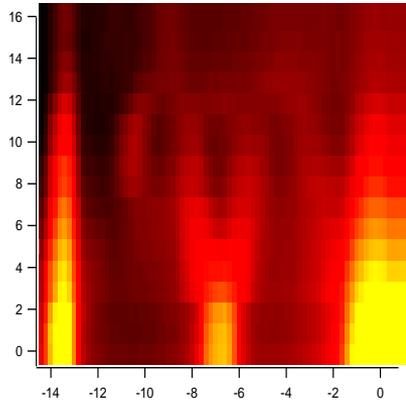
The cell is asymmetric



Asymmetric molecule orientation

The CuPc/Au(110) system

The $\times 5$ phase

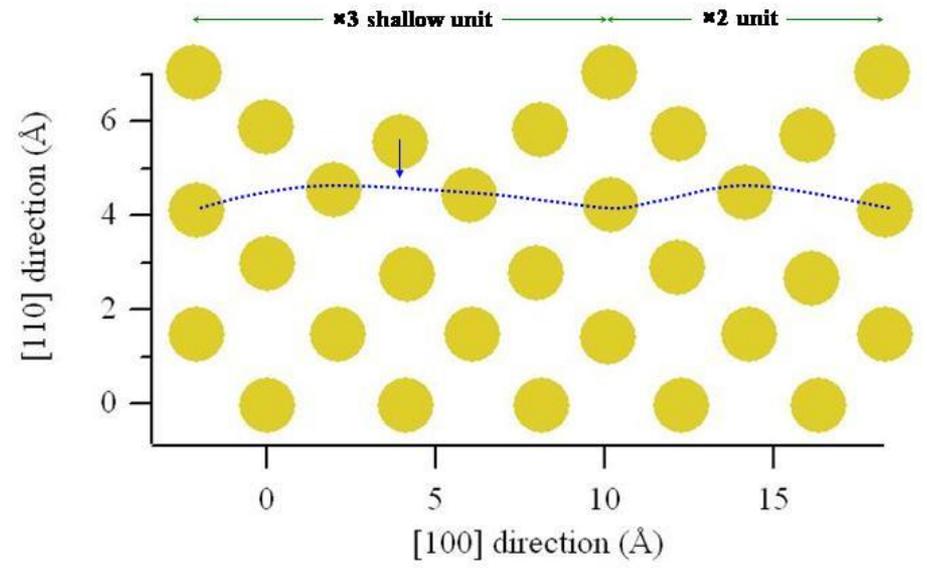
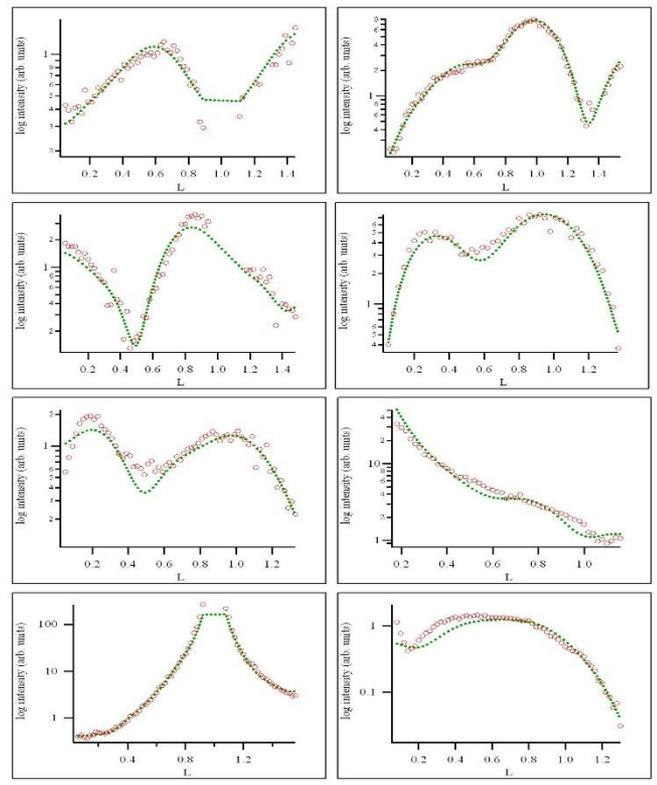


$\times 3$ phase

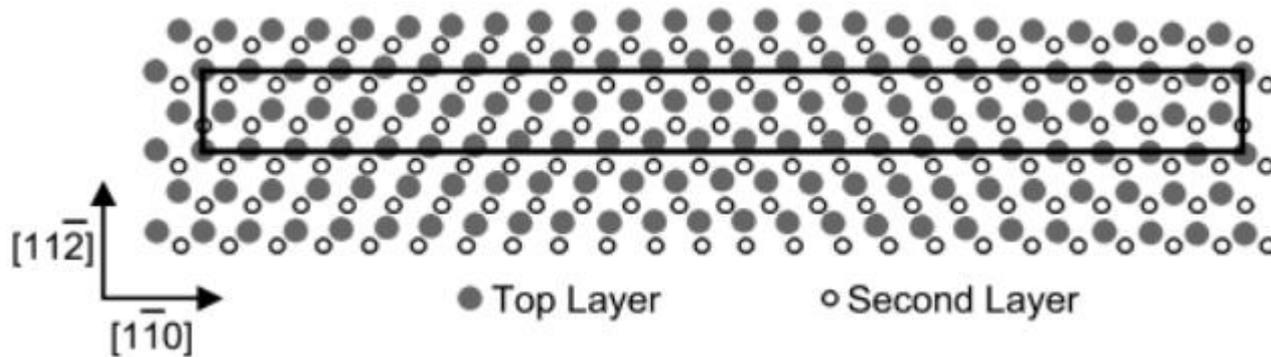
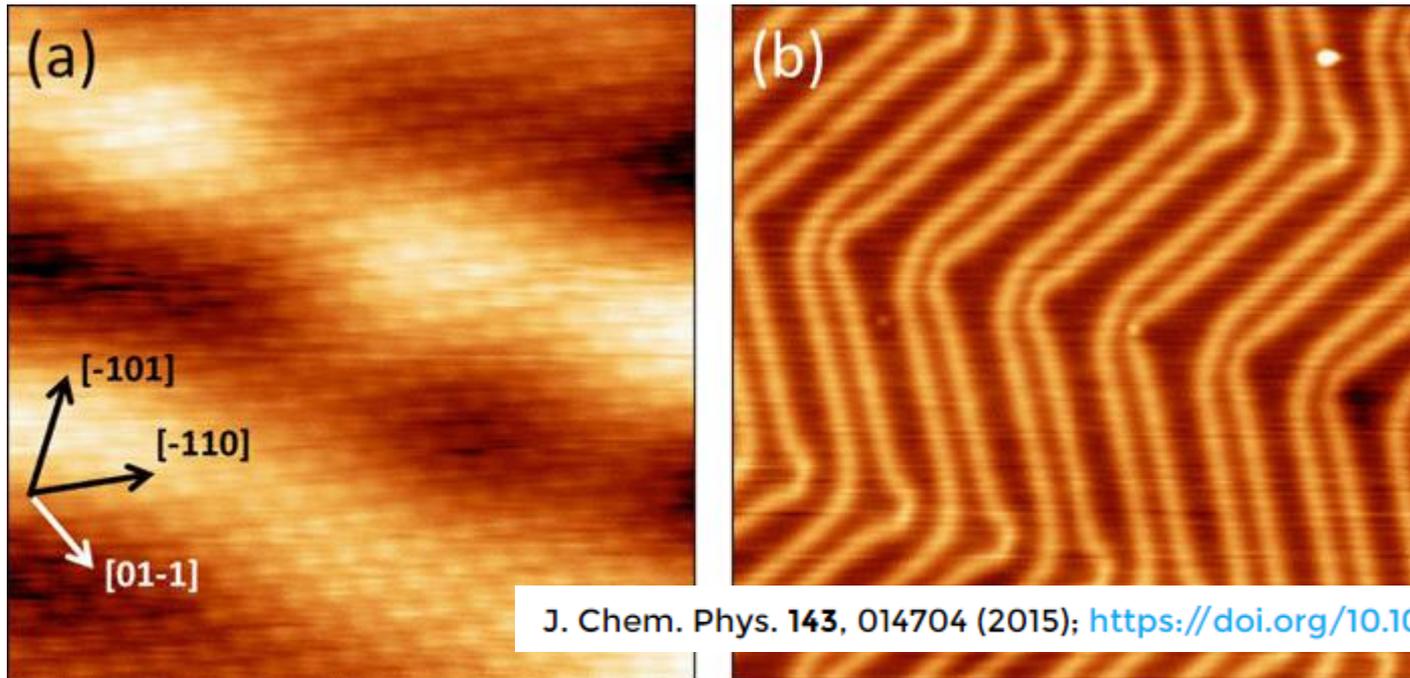
$\times 5$ phase

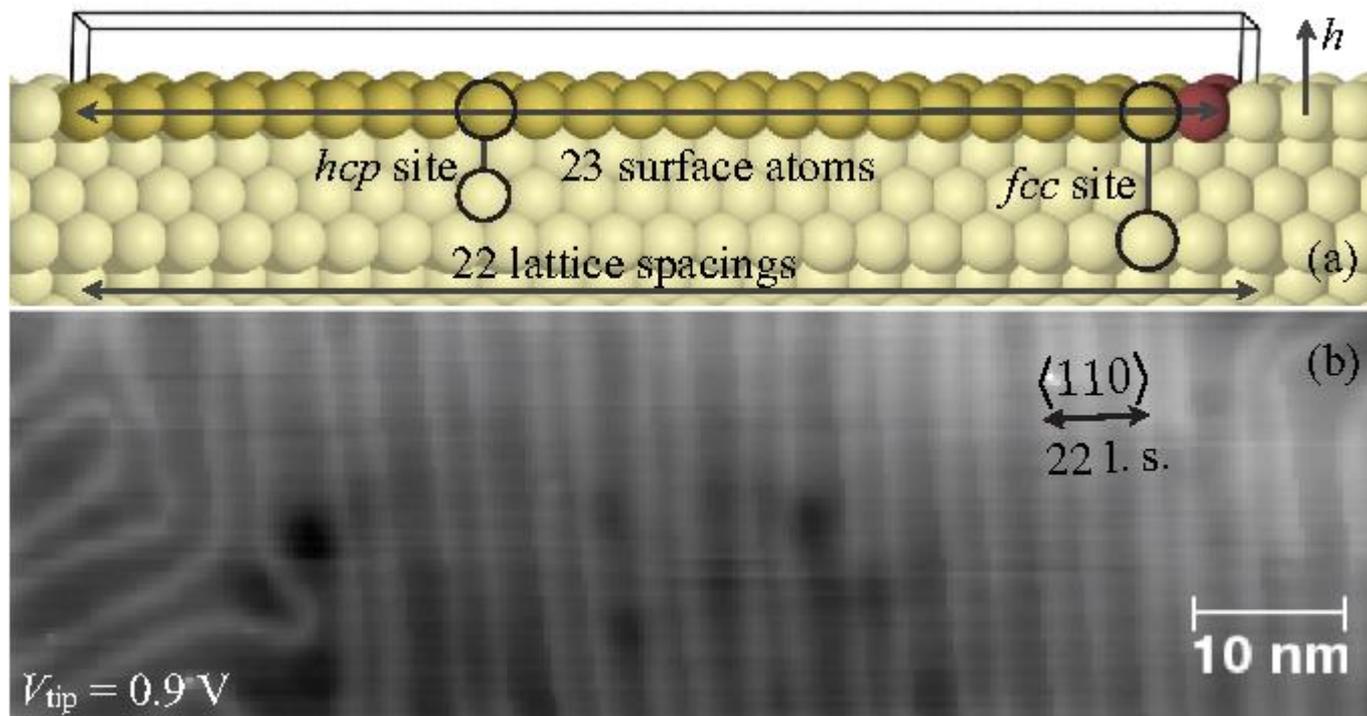
$\times 2$ substrate phase

- Shallow reconstructed $\times 5$ cell
- Junction of $\times 3$ and $\times 2$ cells
- Buckling of the third layer

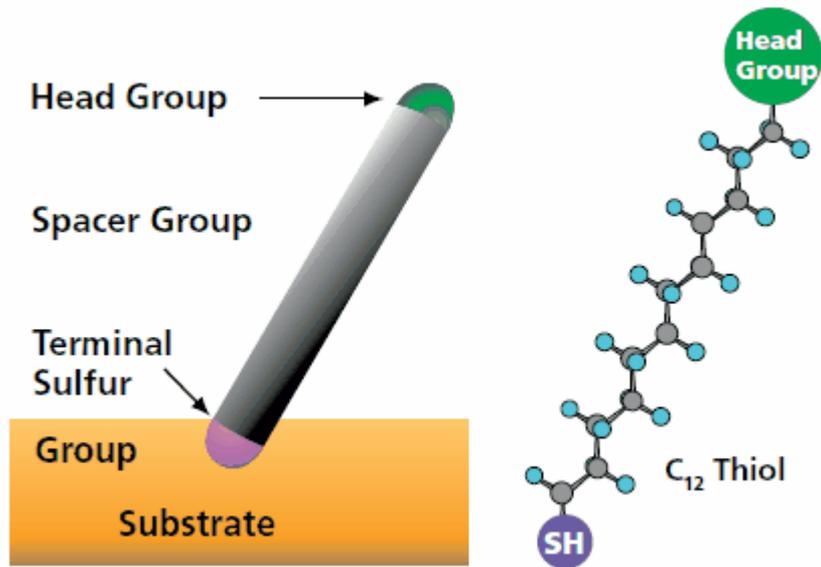


La superficie Au(111): ricostruzione herringbone





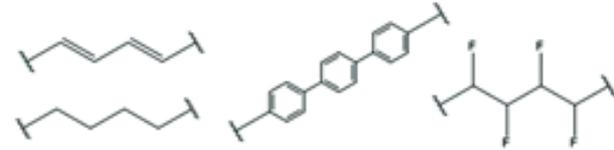
Self Assembled Monolayers (SAMs)



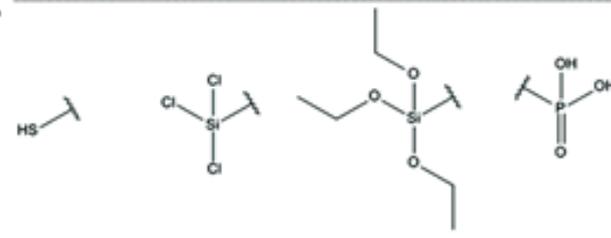
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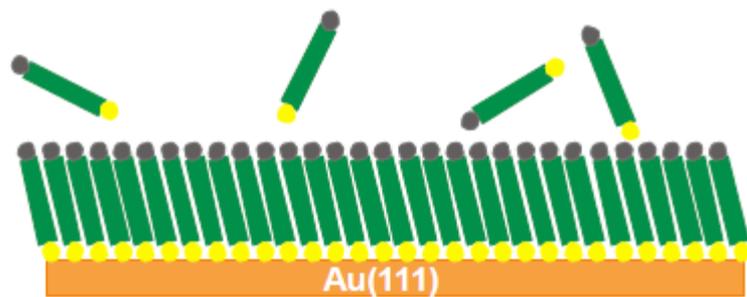
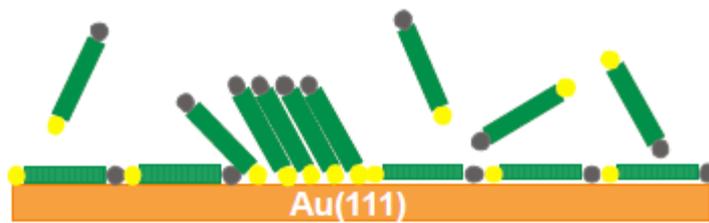
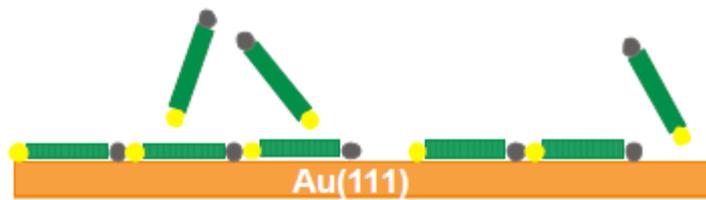


2.



3.





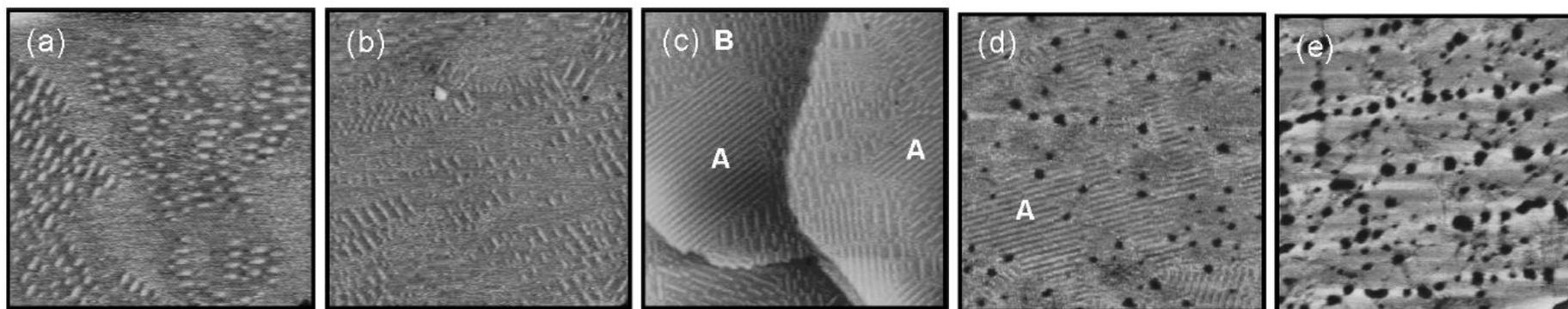
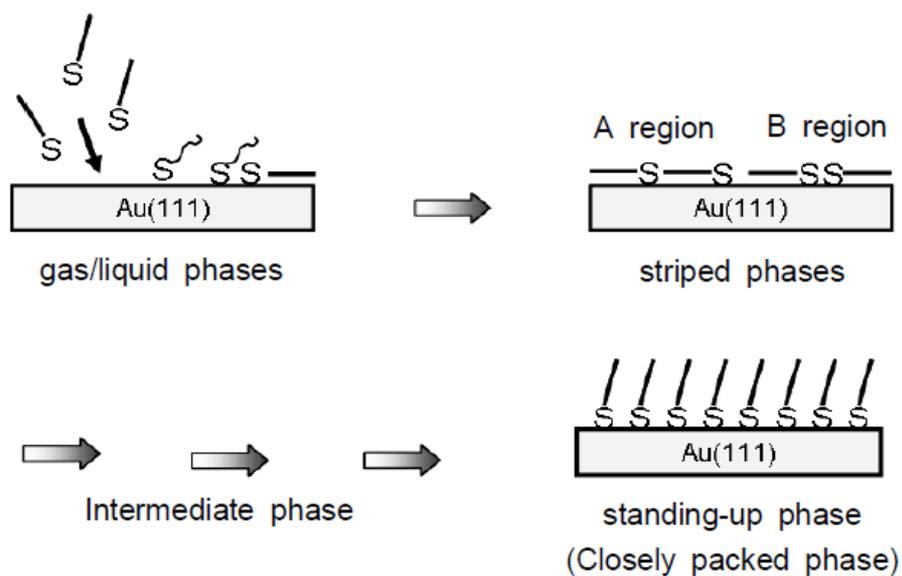
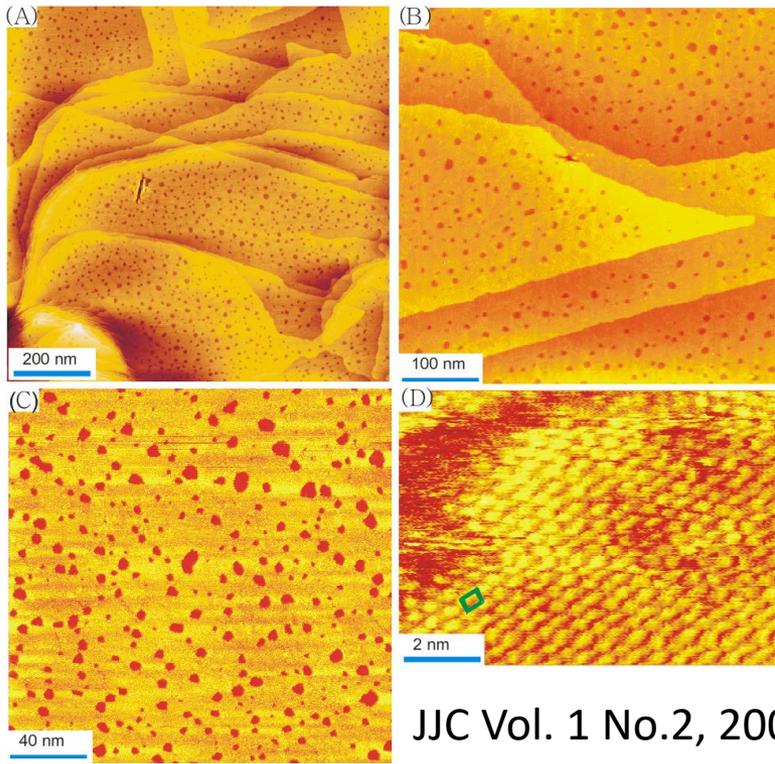


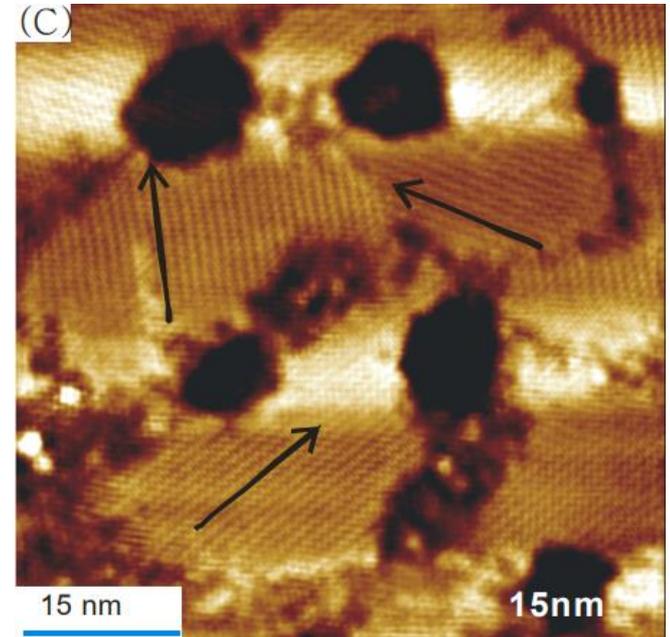
Figure 1. STM images showing the growth process of HDT SAMs on Au(111) after immersion of Au(111) surfaces in a 1 μ M solution as a function of immersion time: (a) 1 min, (b) 5 min, (c) 10 min, (d) 30 min, and (e) 24 h. The scan size of all STM images is 120 nm \times 120 nm.

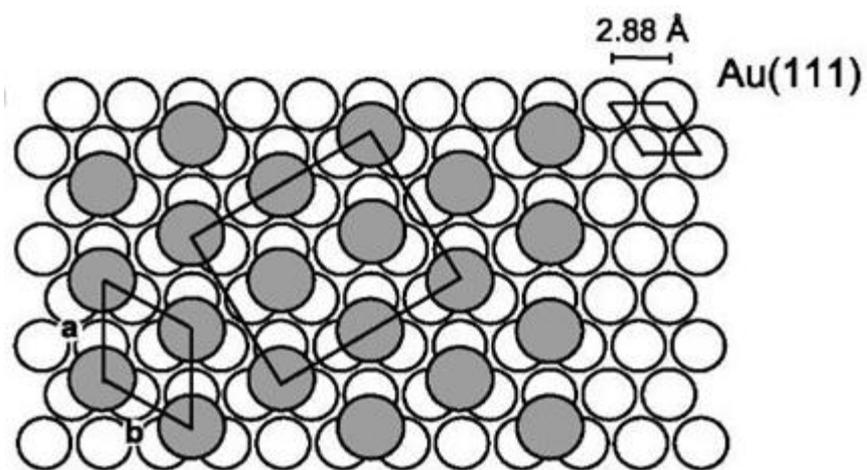
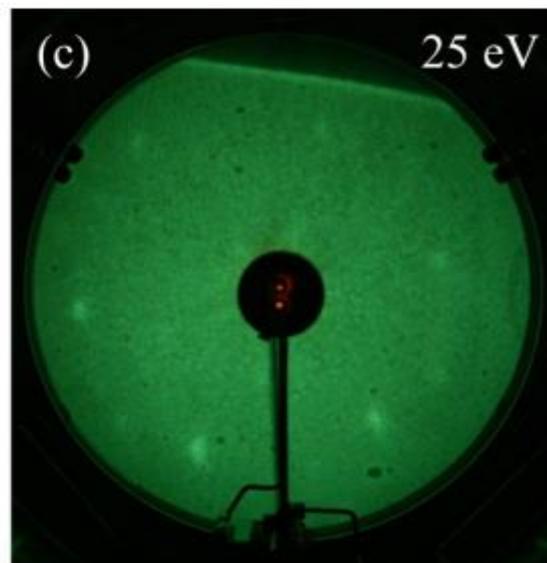
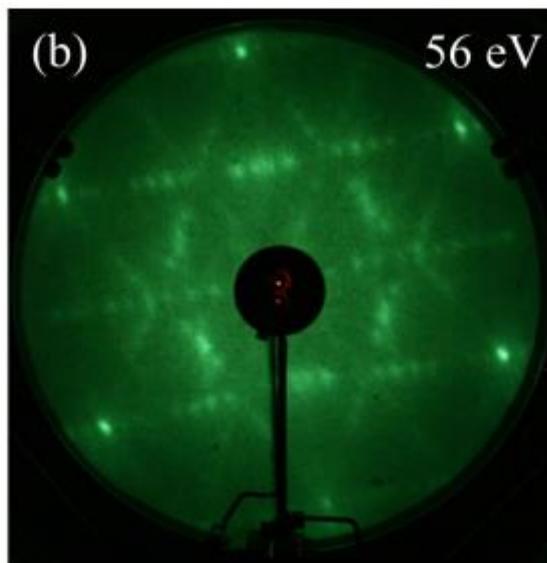
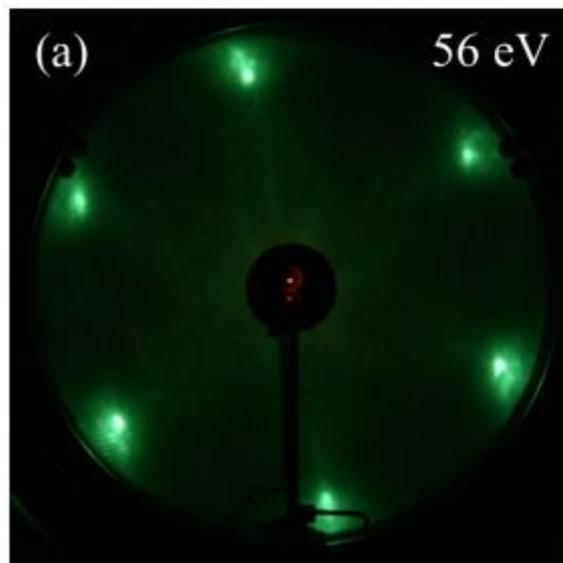


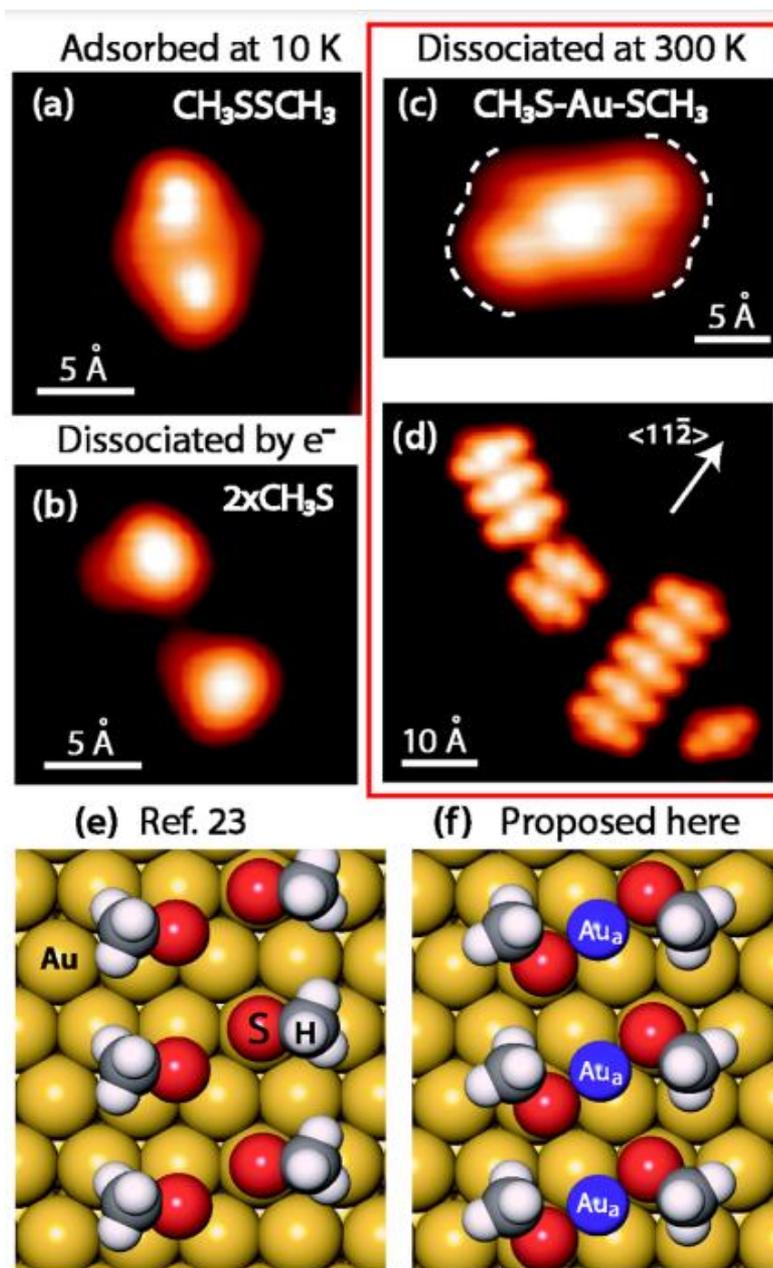
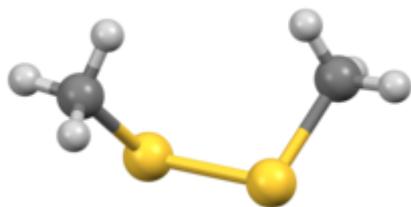
SAM di C10 ottenuto con immersione in soluzione di etanolo per 24 ore

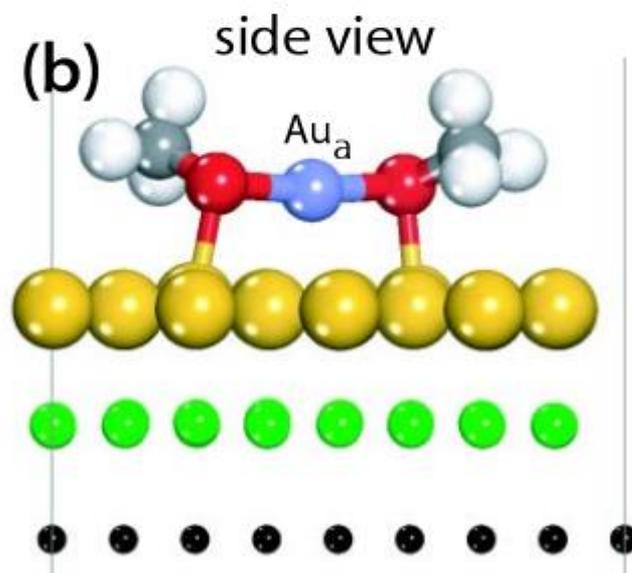
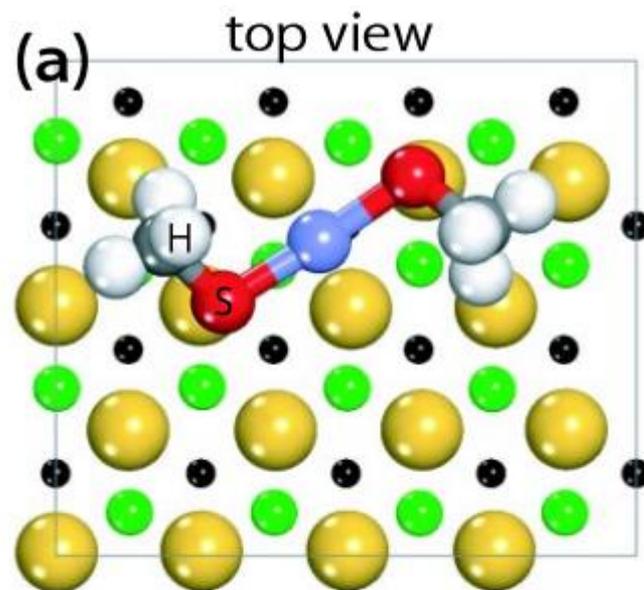


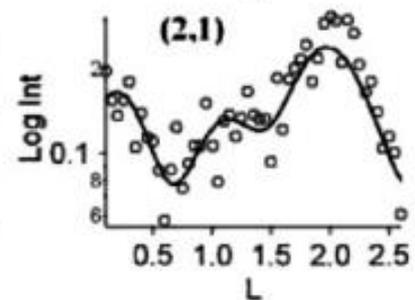
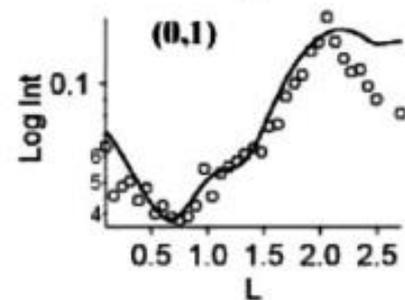
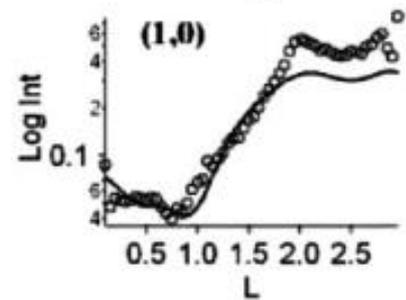
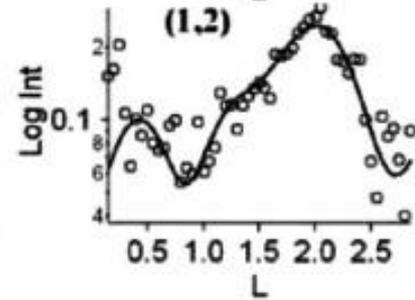
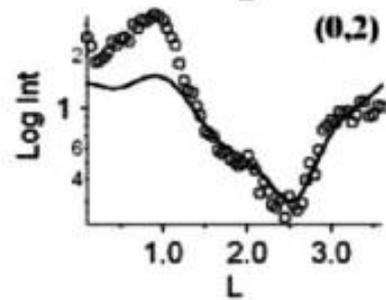
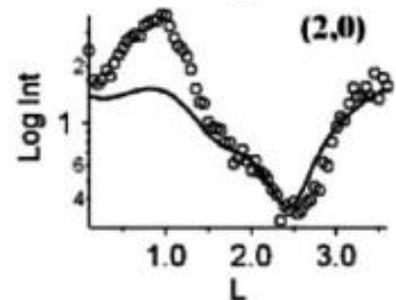
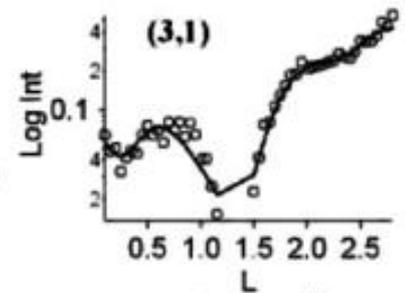
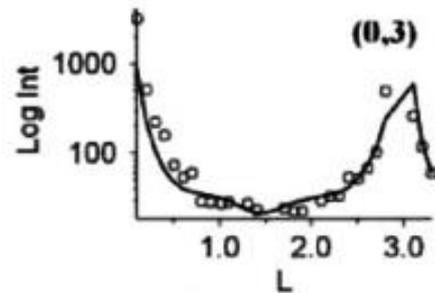
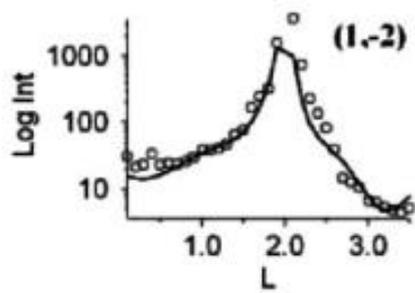
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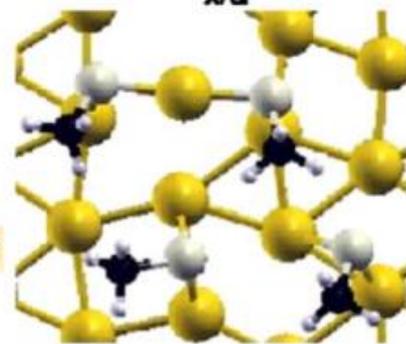
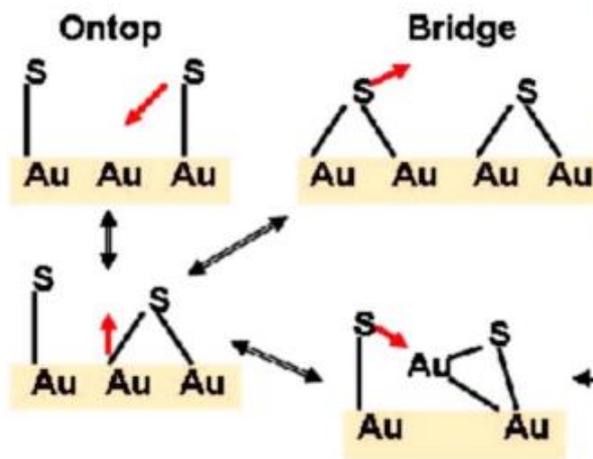
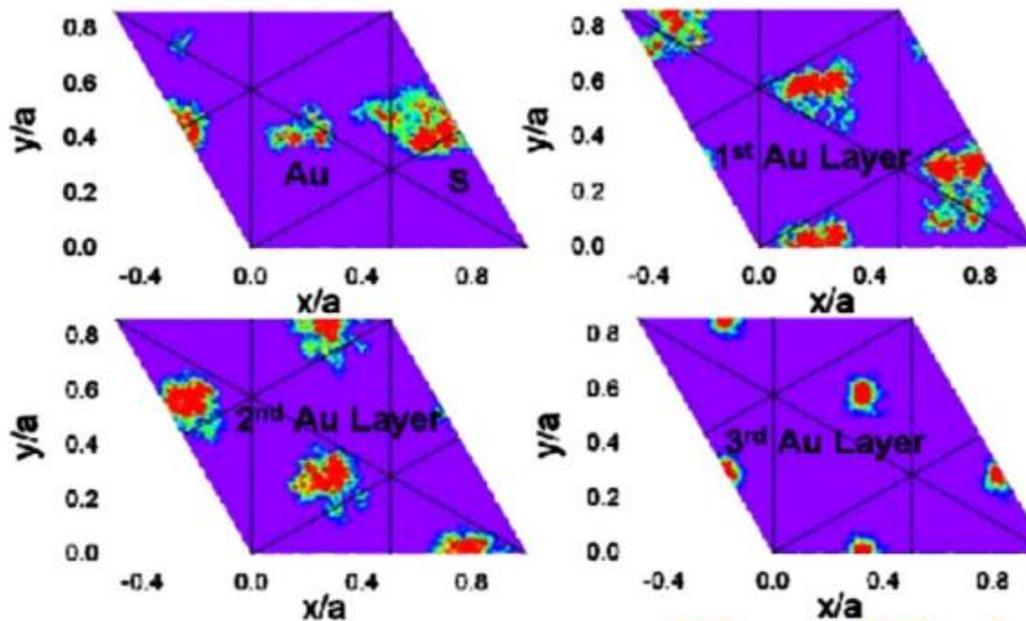


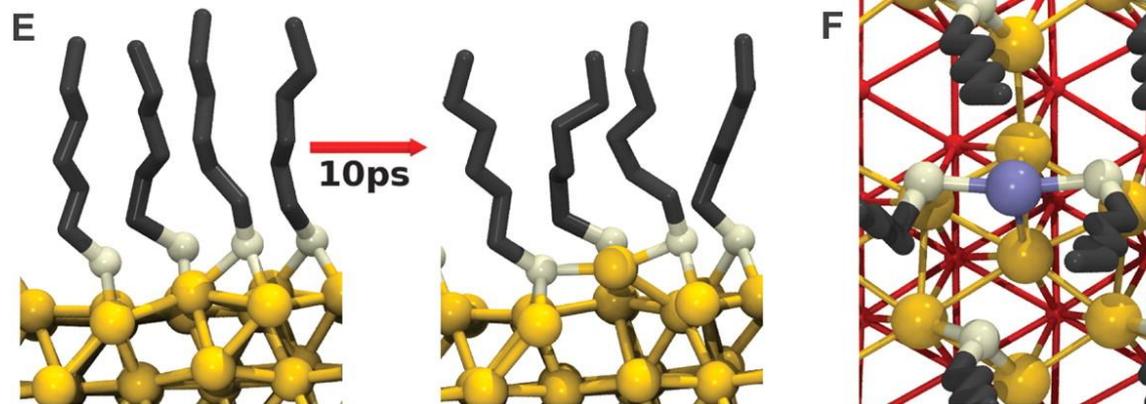
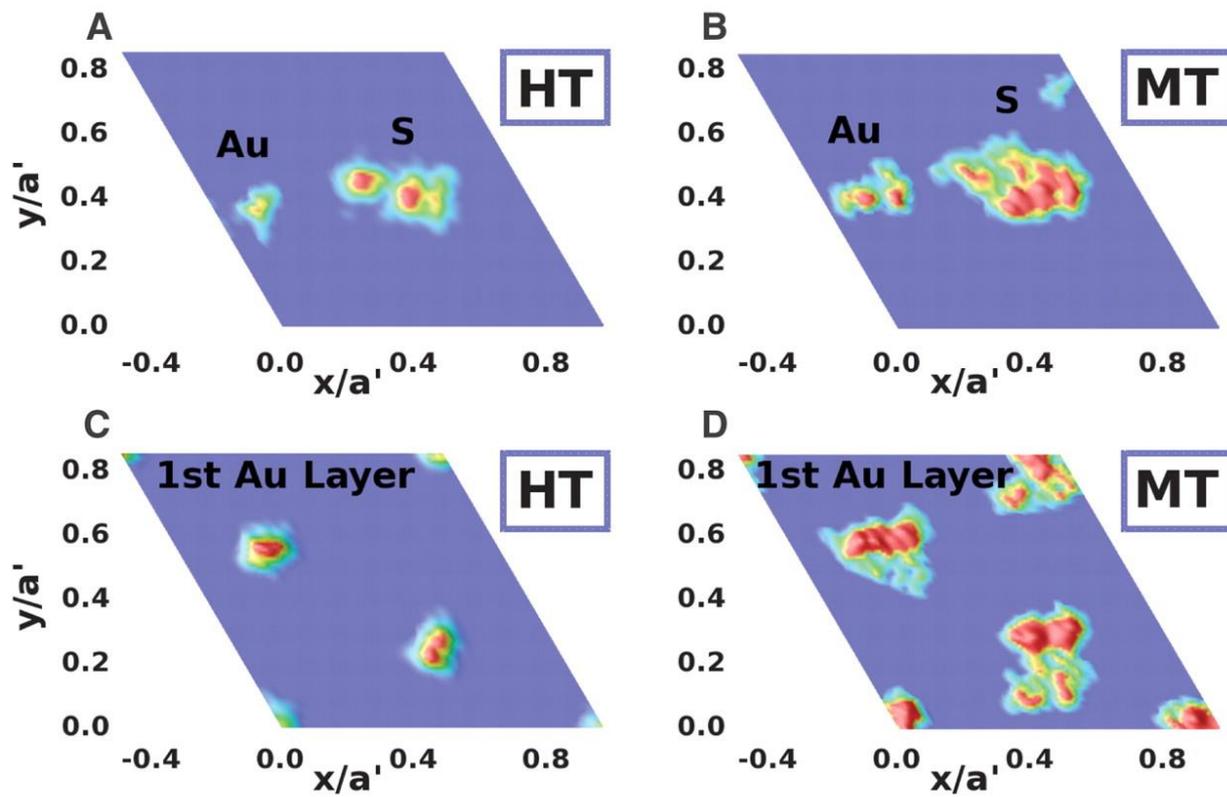


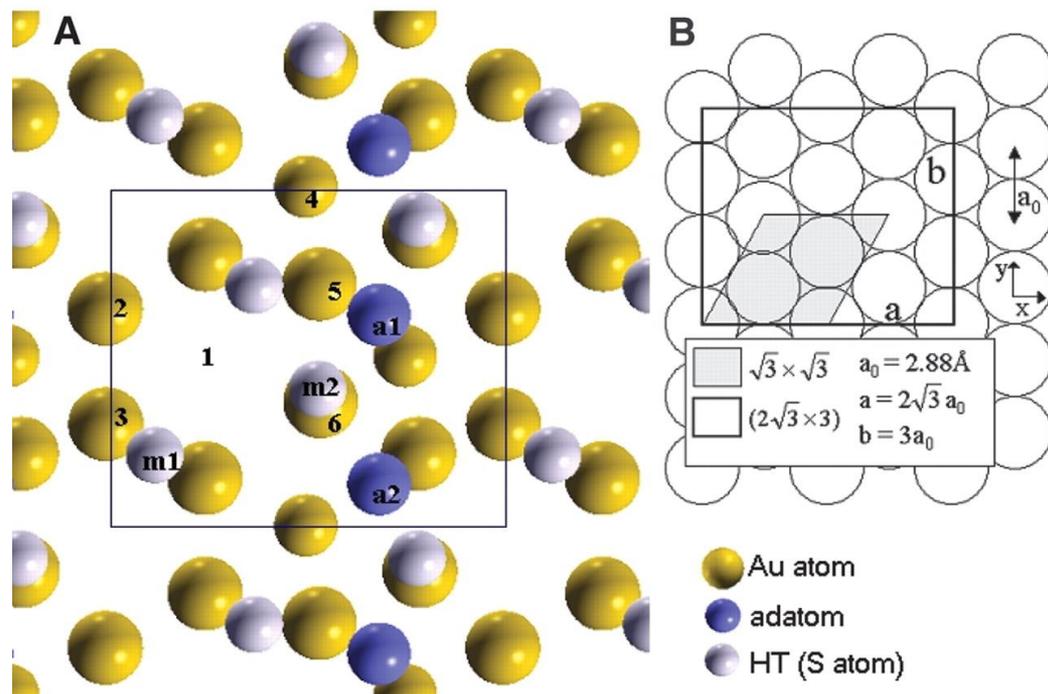
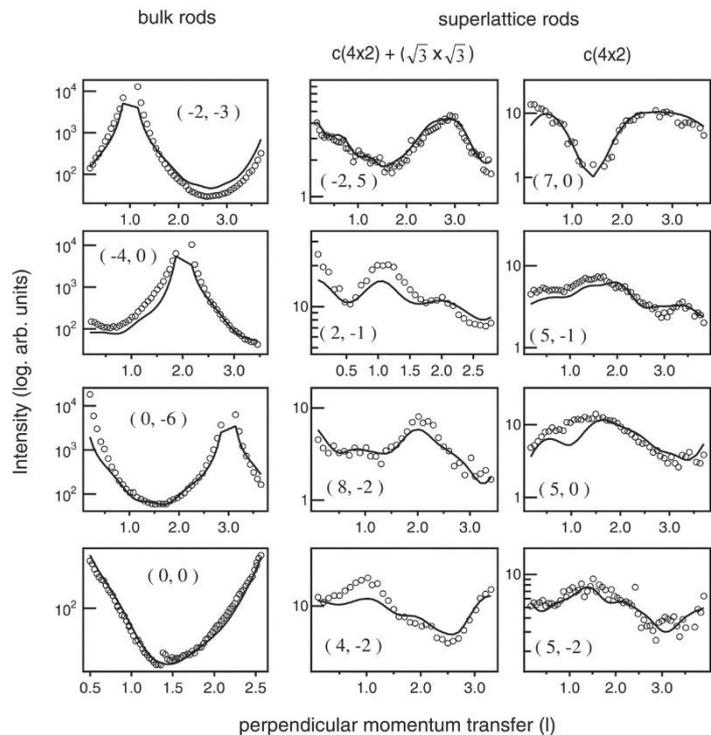






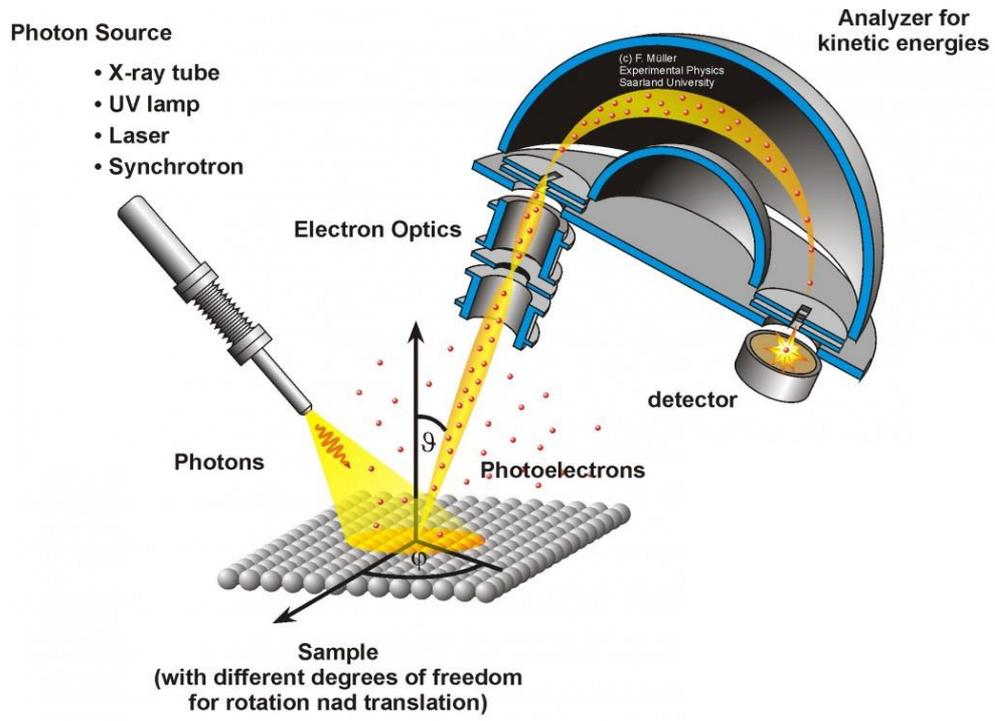






L'analizzatore di elettroni emisferico





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